Recent developments in peridynamics modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A FINITE DEFORMATION MICROPOLAR PERIDYNAMIC THEORY AND ITS APPLICATION TO METAMATERIALS

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ABSTRACT

Metamaterials with engineered microstructures exhibit exceptional properties such as negative Poisson's ratio, energy absorption, and bandgap. Metamaterials find applications in mechanical filter, vibration isolators, biosensor etc. These materials can prevent propagation of elastic waves in certain range of frequency called bandgap. Researchers have developed various novel unit cell configurations to absorb elastic energy and create frequency bandgap. Golub et al. [1] observed that cracks act as reflectors of elastic waves. The microstructure of these materials affects the overall response of the structures. Microstructures may undergo large rotations and their rotary inertia needs to be considered along with deformation. Micropolar continuum theory is developed to address this issue that considers microrotation independent of displacement degree of freedom. The micropolar continuum considers the effect of microstructure by defining the micro-rotation at every material points. However, it is not suitable to analyze the discontinuities as it involves partial differential governing equations. Peridynamics (PD), a nonlocal continuum theory, has integro-differential governing equations which can handle the discontinuities in the structure. As the metamaterials in the study involve cracks, we developed a finite deformation micropolar PD theory to analyze their response. We proved the variational consistency of the wryness measure in an alternative way than the one proposed by Pietraszkiewicz and Eremeyev [2]. A new bond breaking criterion is introduced that uses critical stretch and critical relative rotation. The proposed PD micropolar theory is validated by comparing the results obtained from the boundary element solutions of plate with hole. The response of metamaterials with periodic arrangement of holes and cracks is studied under static and dynamic loads and the results are compared with the nonpolar PD theory.

Keywords: Peridynamics; Micropolar; Metamaterial; Cracks

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Imaging and computational methods for biomechanics
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COMPUTATIONAL APPROACH TO NON-INVASIVELY ASSESS VELOCITY IN ARTERIES FROM CT PERFUSION IMAGING

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ABSTRACT

Introduction
Coronary computed tomography angiography (cCTA) can provide detailed anatomical visualizations of the coronary vasculature to detect diseased coronary arteries (heart vessels). However, not all disease coronary arteries limit blood flow to the heart muscles and thus over-treatment, either with stenting or heart surgery, is common. For targeted treatment, it is necessary to develop methods that can non-invasively detect coronary hemodynamics. One approach to measure blood flow is through CT perfusion imaging, which has conventionally been applied to measure blood flow in the myocardium, but can potentially be used to measure coronary blood flow [1], [2]. Towards this goal, we have developed a computational framework to assess velocity from simulation of contrast perfusion under a range of flow conditions (laminar and quasi-turbulent).

Methods
High-resolution CFD simulations were performed in an idealized, non-axisymmetric stenosis with 75% area reduction. Reynolds number was varied from 100 to 1000 (increment=100) to capture both laminar and turbulent flow regimes. The eccentricity in the stenosis served to destabilize the flow. Advection-diffusion equation was solved with a contrast-bolus curve to simulate the perfusion of contrast into the vessel. Since CT perfusion imaging suffers from coarse spatial resolution and noise, especially near lumen boundaries, it is challenging to estimate the complete three-dimensional velocity field from contrast perfusion. Hence, we assumed unidirectional flow with minimal radial dispersion of contrast to estimate average velocity across the lumen using the following relation: $V=(dC/dt)/(dC/dx)$, where V, C, t and x represent lumen velocity, contrast, time and axial location.

Results
estimated velocity was compared to the assigned mean velocity in the CFD simulations. Error ranged from 0.1 to 9.25 % in the mean velocity for different Reynolds numbers. The contrast transit delay ranged from 46 to 65% of the simulation run-time. The correlation coefficient for estimated velocity vs. calculated velocity was 0.999 and the correlation coefficient between estimated velocity and transit delay is -0.9305.

Discussion and Conclusion
Despite flow-regime dependent errors, our study demonstrates the feasibility of estimating lumen velocity using contrast perfusion imaging. Notably, estimated velocities closely mirror CFD simulations at all Reynolds numbers (errors < 10%). Furthermore, higher Reynolds numbers exhibit shorter simulation times and lower relative errors. This agreement across diverse flow conditions underlines the robustness of our method.

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Deep and machine learning methodology in the context of application to computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CONVOLUTIONAL VARIATIONAL PHYSICS-INFORMED NEURAL NETWORKS TO SOLVE A FINITE ELEMENT FORMULATION

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ABSTRACT

We propose an extension to physics-informed neural networks (PINN) in which the outputs of the network are used to approximate the weak-form residuals of time-dependent partial differential equations (PDE) using convolution operations. PINNs are machine-learning methods that leverage the physics expressed in the PDEs to extract information from high-dimensional data generated through experiments. They received considerable attention in the literature due to their approximation capabilities and effectiveness in solving forward and inverse linear and nonlinear PDEs. Resembling the finite elements method (FEM), the current variational physics-informed neural networks (hp-VPINN) formulate the solution based on domain decomposition and projection onto space of high-order polynomials allowing the network to construct both global and local approximations. The weak-form residuals of the equations of each sub-domain are then approximated using the Gauss quadrature rule sequentially, where the network is trained to minimize those residuals. However, the computation cost of the current hp-VPINN escalates drastically when the domain is discretized into a few sub-domains, not to mention many subdomains. This limits the ability of hp-VPINN to approximate the solutions when dealing with complex problems requiring many elements or sub-domains. Using convolution operations to evaluate the Gauss quadrature sum allows for parallelization in evaluating the weak-form residuals of the sub-domains which significantly improves the computation efficiency. By incorporating customized test functions and the integral weights within the convolution filters and multiplying them across the network outputs to evaluate the weak-form residuals, we demonstrate that convolutional PINNs achieve three orders of magnitude higher precision in predictions than PINNs. Furthermore, they converge nine times faster than hp-VPINN when solving the one-dimensional wave equation. We also show that this extension enables us to use smaller-sized networks, which further improves the computation speed. In addition, we illustrate the efficacy of the convolution PINN in solving inverse problems related to the one-dimensional wave equation and the linear pipe conveying fluid equation. Ultimately, we plan to extend the application of convolution PINN to higher dimensional problems for both the two-dimensional wave equation and the three-dimensional nonlinear pipe conveying equations. This formulation blurs the line between the conventional finite element method and AI methods as it makes use of neural networks to solve an FEM formulation.

Numerical modelling of composite materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREDICTION OF THE FAILURE BEHAVIOR OF PSEUDO-DUCTILE COMPOSITES USING A MICRO-MECHANICAL FINITE ELEMENT MODEL

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ABSTRACT

The hybridization technique has recently been used to produce a new generation of composites called pseudo-ductile composites, which have shown higher failure strain compared to conventional composites, minimizing the risks of the occurrence of a catastrophic failure. The pseudo-ductility behavior in these composites is obtained by hybridization of fibers with high and low failure strains.
In this study, a micro-mechanical finite element (FE) model is proposed to predict the failure behavior of pseudo-ductile composites with conventional thickness. A representative volume element (RVE), consisting of randomly distributed fibers, was generated using a Python code. Mechanical properties, including elastic and failure constants, were assigned to the fibers and matrix. To account for fiber failure and ply fragmentation, the tensile strength of fibers was distributed based on the Weibull distribution function. Tensile loading was then applied to the RVE to simulate the composite's mechanical behavior using FE analysis.

To validate the numerical model, an RVE was developed based on the experimental data obtained from a recent research on conventional thickness composites. The numerical results were compared to the experimental data, showing acceptable agreement.

The effect of fiber volume fraction in the low-strain ply on the tensile mechanical properties of pseudo-ductile composites was investigated. In addition, the influence of the Weibull modulus on the composite's mechanical behavior was evaluated through a sensitivity analysis. Lower Weibull modulus values resulted in linear behavior, while higher values yielded nonlinear stress-strain curves. Notably, high Weibull modulus values exhibited a sudden stress drop, indicative of diminished pseudo-ductile behavior.

Overall, this research provides valuable insights into the prediction and analysis of the tensile mechanical response of pseudo-ductile composites. The proposed numerical model showcases promising agreement with experimental results, validating its efficacy. Understanding the impact of fiber volume fraction and Weibull modulus contributes to the optimization and design of these composites, facilitating their implementation in various applications.

Data-driven modeling and design of materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VISCOELASTIC CONSTITUTIVE ARTIFICIAL NEURAL NETWORKS (VCANNS) - A FRAMEWORK FOR DATA-DRIVEN ANISOTROPIC NONLINEAR FINITE VISCOELASTICITY

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ABSTRACT

Finite linear viscoelastic or quasi-linear viscoelastic models are commonly used to model the constitutive behavior of polymeric materials [1]. However, these models' limitations in accurately describing nonlinear viscoelastic phenomena, particularly in capturing strain-dependent viscous behavior, motivate the development of alternative methodologies. In response to this issue, we introduce viscoelastic Constitutive Artificial Neural Networks (vCANNs) [2], a novel physics-informed machine learning framework. vCANNs rely on the concept of generalized Maxwell models with nonlinear strain (rate)-dependent properties represented by neural networks. With their flexibility, vCANNs can automatically identify accurate and sparse constitutive models for a broad spectrum of materials. To assess the capabilities of vCANNs, extensive training was conducted using stress-strain data from synthetic and biological materials subjected to diverse loading conditions, e.g., relaxation tests, cyclic tension-compression tests, and blast loads. The results show that vCANNs can learn to accurately and efficiently represent the behavior of these materials without human guidance. We showcase the seamless integration of vCANNs into existing finite element codes through illustrative examples. This integration underscores the practical applicability of vCANNs in applied mechanics.

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MODELING AND SIMULATION OF THERMAL DEGRADATION IN A COMPOSITE MATERIAL SUBJECTED TO HEAT FLUX

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ABSTRACT

Keywords: Composite materials, microstructure, pyrolysis, thermal degradation, interface, coupling, gradient-based model, phase field

Composite materials are widely used in structures where weight reduction is crucial while maintaining high stiffness and strength properties. Under strong thermal stress, these materials degrade and alter their physical properties [1]. In order to understand and enhance the fire behavior of these materials, the objective of this study is to establish a numerical model at microstructure scale to simulate the thermal degradation (pyrolysis decomposition) of a composite material subjected to a heat flux. A rigorous thermodynamic approach with internal variables has been adopted to better capture the phenomenon under study. In the literature, the models used to describe this degradation generally do not take into account the influence of microstructural heterogeneity on the decomposition rate, on the degradation kinetics and, consequently, on the propagation of the thermal front decomposition. To consider the variability of the composite microstructure, simulations at the microscale were conducted, involving a strong coupling between the evolution of the thermal degradation rate (which follows an Arrhenius law) and the temperature evolution using the phase-field method. This method is suitable for simulating phase transition phenomena and interface motion in a non-homogeneous material [2][3]. This approach introduces a degradation gradient term to characterize the interface energy between degraded and sound regions, allowing the influence of microstructural fluctuations to be considered.
Experimental tests were conducted to identify the input parameters of the model and to validate it. Firstly, observations using an optical microscope are carried out to reconstruct the microstructure, which is essential for a reliable simulation. Then, a post-processing is performed to delineate the distinct phases of the material. Secondly, characterization tests, such as thermogravimetric analysis (TGA), have been conducted to identify model parameters. Finally, we carried out cone calorimeter tests to compare the results with the numerical simulations. This comparison focuses on the analysis of the degradation kinetics as well as the evolution of the mass loss.

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DISCOVERY OF ASYMPTOTIC EXPANSIONS OF MECHANICAL PROBLEMS USING SYMBOLIC REGRESSION

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ABSTRACT

Asymptotic methods play an important role in a wide variety of physical problems, including the analysis of thin plates and shells, the solution of the Navier-Stokes equation, and the propagation of elastic waves in highly inhomogeneous structures, see, e.g., [1,2] and references therein. In many cases, it is challenging to identify the effect of small problem parameters and to derive their asymptotic expansions of the desired solution. Recently, data-driven methods such as symbolic regression have demonstrated their high efficiency in discovering equations and physical relationships [3].

This work proposes a new automatic method for generating asymptotic expansions based on symbolic regression. The goal is to find an asymptotic series in a form that fits the given analytical solution as closely as possible. Therefore, data is generated from analytical solutions for a chosen small or large parameter. First, a two-mass collision problem is discussed for three boundary scenarios. Subsequently, a divergent asymptotic series resulting from the implementation of a viscoelastic Kelvin-Voigt model is investigated. Finally, Lamb waves propagating in an elastic layer are studied. Good agreement between the asymptotic expansions obtained by symbolic regression and the underlying analytical solutions is demonstrated.

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Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GRID-PARTICLE COUPLING SIMULATION FOR SLD ICING INTRODUCING HIGH-RESOLUTION SCHEME AND IMPROVED THERMODYNAMICS COMPUTATION

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ABSTRACT

Ice accretion is the phenomenon that forms an ice layer when supercooled droplets impinge on a body and occurs in several situations in the industrial field. Particularly, icing on aircraft poses a threat to navigation safety because the ice layer can alter the airflow around the wing and deteriorate aerodynamic performance. Given that aircraft are equipped with anti- or de-icing systems to avert serious accidents, accurate prediction of aircraft icing is essential during the design phase of the systems. Despite extensive research, the methodology for the detailed icing simulation has not yet been established due to the challenges posed by multi-physics problems. In addition, under the conditions involving supercooled large droplet (SLD), where the diameter of droplets in the cloud exceeds 40 μm, the splashing and the rebounding of droplets generate secondary droplets. These factors contribute to the increased complexity of the ice shape and render the prediction of icing more challenging. This study suggests a pragmatic simulation approach to address the trade-off issue between high-resolution simulation and computational cost. We utilize a coupling scheme involving grid- and particle-based methods; the grid-based method is employed for computing the flow field and the droplet trajectory, while the particle-based method is utilized for determining the behavior of impinged droplets and the icing process. The particle-based method can reproduce the distinctive phenomena of SLD without relying on empirical models, as it facilitates the direct computation of droplets' impingement behavior. On the other hand, this method incurs significant computational costs when simulating large-scale phenomena with high spatial resolution. Therefore, we propose a method that reduces computational cost with accuracy. This approach minimizes the simulation cost, and the ice shape is extrapolated based on the increasing ice mass ratio. In the computation of the icing process, we accounted for both conductive heat transfer within the ice or water layer and convective heat transfer between the airflow and ice surface. To account for the change of the airflow by ice, we introduced a multi-shot simulation, updating the flow field and the droplet trajectories over time. Employing these methods, we performed a two-dimensional simulation of SLD icing on the NACA0012 airfoil. As a result, the computation for actual scale can describe a more complex ice shape, with the ice mass increasing due to heightened heat flux caused by convective heat transfer. The present method offers a more practical and precise simulation approach for addressing aircraft icing issues.

Phase-field models of fracture
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RATE DEPENDENCY OF INTERFACIAL AND BULK FRACTURE MODELS

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ABSTRACT

We will examine the rate dependency of several fracture models from two perspectives: 1) The form of differential equation and damage driving force, especially the temporal derivatives of the equation; 2) Instabilities that arise as damage localizes in 1D to 3D problems. For the first aspect, we present elliptic, parabolic, and hyperbolic forms of a phase field formulation. In a so-called 0D model, we assume that the solution fields do not vary in space. We then demonstrate that maximum stress and fracture energy of the elliptic model are rate-independent. The parabolic and hyperbolic models are both rate-dependent with the difference that the hyperbolic model exhibits a higher sensitivity. We also relate this work to other differential equations that arise in fracture namely bulk and continuum damage models. Using the asymptotic expansion method, we demonstrate that the form of the damage driving function also influences the extent of rate dependency. For example, energy-based models exhibit a lower rate-sensitivity than effective stress-based models.

For the second aspect, i.e. rate-dependency arising from damage localization, we show such effect exists even for the rate-independent 0D model; that is, for the elliptic PDE. We compare the responses of 1D and 0D models as well as hyperbolic / elliptic differential equations with the elliptic equation in 1D. For these 1D fracture simulations, we also examine the effect of material heterogeneities on macroscopic Quantities of Interest (QoIs) such as maximum stress, dissipated energy, and fragment statistics. Finally, we will present machine learning models that are trained to predict these QoIs from key loading and nondimensional material parameters, as well as a low dimensional representation of the underlying heterogeneous material property field.

High order methods for time-dependent problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NATURAL FREQUENCY AND DISPERSION ANALYSIS OF CONTINUOUS AND DISCONTINUOUS GALERKIN METHODS FOR 1D WAVE EQUATION

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ABSTRACT

This study presents a comparison of the dispersion and dissipation of various 1D finite element formulations for the wave equation. The study includes continuous finite elements (CFEM), Symmetric Interior Penalty Galerkin (SIPG), Nonsymmetric Interior Penalty Galerkin (NIPG), and Incomplete Interior Penalty Galerkin (IIPG) methods. For the Discontinuous Galerkin (DG) methods, three different weak formulations with different primary fields have been considered: displacement, velocity, and two fields simultaneously. In addition, the calculation of the numerical flux is conducted with Reimann, central, and alternating methods. The eigenvalue problem of the free vibration is used for the dispersion analysis using the duality principle [1]. Spectral analysis has been conducted for different polynomial orders and penalty values. The results indicate that the penalty values for the central flux approximation have an optimal value for both primary fields, and the central method provides more accurate results than the Reimann solver when that optimal value is used for the penalty. In addition, DG formulations can have better approximations than the CFEM, depending on the penalty values. Overall, for all the formulations that are considered, increasing the polynomial order also decreases the error. Even though there are some trends observed when changing the penalty values or the polynomial order, the accuracy of a given method highly depends on the wave number, and different methods can have different performances depending on the considered spectral window.

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Data-driven methods for modeling complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DYNAMIC VIBRATION ABSORBER WITH HYDRAULIC AMPLIFIER AND MECHANICAL INERTER: A NOVEL APPROACH

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ABSTRACT

To enhance the performance of the Dynamic Vibration Absorber (DVA) amplification mechanism is proposed to overcome the limitations associated with the mass ratio in passive DVAs with a mechanical inerter which enhances the damping. Traditional lever amplification mechanisms encounter challenges with length ratio and rigidity, especially in large-scale systems. The novelty of the proposed system lies in integrating a DVA with a Hydraulic Amplifier (HA) and a mechanical inerter, exploring various configurations. Additionally, piezoelectric elements for energy harvesting is incorporated. The main issue encountered with HA is fluid friction loss, which is inversely proportional to the diameter of the HA. However, increasing the diameter also escalates weight and cost. To address this, Differential Evolution (DE) optimization to minimize friction loss and pipe weight is developed and implemented. Using a large dataset from optimization runs, an Artificial neural network (ANN) to predict optimal HA dimensions is trained, tested, and validated. Further optimization aims to minimize vibration while maximizing output voltage, using Multi-objective Weighted Sum Particle Swarm Optimization (PSO) and Genetic Algorithm (GA). Our findings indicate that the amplification process not only enhances damping but also broadens the frequency band. PSO solutions generally outperform GA solutions in terms of diversity and quality, although we observe fluctuations in PSO solutions' stability compared to GA solutions under corresponding weight settings.
The proposed model of the DVA with HA and mechanical inerter successfully compensates for the limitation of the mass ratio required to increase the damping and it increases the working frequency band of the DVA. Multi-objective optimization using PSO generally outperforming GA in diversity and quality, although fluctuations in stability have been observed in PSO. The train data was used to select the best dimensions of the HA. HA has advantages over the lever amplification, the flexibility of the alignment of the configuration, and the ability to connect different vibrated systems to a single DVA which consequently increases the energy harvested.

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Data-driven approaches for solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A PHYSICS-INFORMED NEURAL NETWORK FOR INVERSE CHARACTERIZATION OF CONSTITUTIVE MODELS USED IN PROGRESSIVE DAMAGE ANALYSIS OF COMPOSITES

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ABSTRACT

Successful simulation of progressive damage and failure response of composite structures relies on accurate characterization of constitutive models that in the macroscopic sense are typically in the form of strain-softening curves. This necessitates conducting high-quality coupon-level experiments coupled with the implementation of efficient inverse strategies for calibration of constitutive model parameters. Conventional inverse methods often involve iterative processes, requiring reruns of numerical models for each parameter update leading to tedious calibration procedures.
This study presents a physically meaningful machine learning approach based on Physics-Informed Neural Networks (PINNs) [1]. PINNs explicitly incorporate the underlying physics of the problem, offering increased interpretability and the ability to train with smaller datasets [2]. We develop a PINN-based framework for characterizing the strain-softening response of composite materials leveraging real-world notched fracture tests. The training dataset for the proposed PINN includes full-field displacement and global force measurements. To overcome the training challenges associated with severe localization in the fracture tests, we design an enhanced architecture by implementing a pipeline of forward and inverse neural networks. The performance of the developed framework is validated using synthetic data obtained from finite element simulations of the fracture tests.
To bridge the gap between theoretical and real-world experiments, our methodology is applied to a series of physical tests on quasi-isotropic IM7/8552 Carbon Fiber Reinforced Polymer (CFRP) composite laminates. Over-height Compact Tension (OCT) [3] and Compact Compression (CC) tests are conducted to promote stable growth of damage in tension and compression, respectively, allowing for the generation of sufficient data in the damage regime of the constitutive model. The full-field displacement data required for PINN training are obtained from experimental measurements using the digital image correlation (DIC) technique. For validation purposes, the PINN-characterized constitutive models are used within the FE simulation of the OCT and CC tests, and the resulting force-POD (pin opening displacement) response curves obtained from the simulations are compared against the corresponding experimental curves.

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DETECTING AND QUANTIFYING STRUCTURAL NONLINEARITIES: A SYNERGISTIC APPROACH USING POST-HOC INTERPRETABILITY AND NEURAL NETWORKS ON RESPONSE SIGNAL TIME SERIES

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ABSTRACT

Abstract:
In the realm of computational mechanics, accurately detecting, characterizing, and quantifying structural nonlinearities remains a pivotal yet challenging endeavor[1]. This study introduces an innovative methodology that synergistically combines post-hoc interpretability[2] with nonlinear parameter estimation via neural networks, leveraging their universal approximation properties.

The robustness and applicability of our method are meticulously validated through a series of numerical test cases, each simulating a single degree of freedom system with inherent nonlinearity.

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Imaging and computational methods for biomechanics
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PSEUDODIFFERENTIAL APPROXIMATIONS OF ULTRASOUND WAVES FOR BIOMEDICAL APPLICATIONS

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ABSTRACT

Computational simulations are playing an increasingly important role to improve therapeutics and diagnostics using ultrasound waves. To unleash the full potential of computer simulations, the computational method must strike the right balance between accuracy and speed. We develop a fast pseudodifferential method that takes advantage of the geometric flow of acoustic energy to efficiently handle the highly oscillatory nature of ultrasound waves. Simultaneously, the method accurately incorporates refraction, reflection and attenuation imposed by realistic models of biological media. As a result, simulations of ultrasound wave propagation can be executed orders of magnitude faster than using conventional approaches. Some numerical results will be presented, and limitations discussed.

Computational mechanobiology of musculoskeletal tissues
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING TARGETED BONE REMODELING AND VOXEL-BASED COMPUTER SIMULATION

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ABSTRACT

Bone with accumulated microdamage due to mechanical loadings is repaired by so-called targeted remodeling. In this process, mechanosensory osteocytes detect the microdamage and signal neighboring cells to activate osteoclastogenesis, initiating resorption-formation-coupled bone remodeling. This process is fundamental to maintaining the mechanical integrity of bone throughout life effectively preventing age- and disease-related loss of bone strength. However, the coupled phenomena of mechanics, such as damage accumulation under loadings, and biology, such as detection and repair of the microdamage by cellular activities, are complex and thus require understanding as a mechanobiological system. In this study, we aimed to model and simulate targeted remodeling by incorporating molecular and cellular mechanisms into the in-silico experimental platform (V-Bone) [1], which enables a voxel-based bone remodeling simulation that incorporates mechanics and biology within a single framework. By introducing a damage variable as a scalar function, microdamage accumulation in the bone matrix under mechanical loadings was modeled, based on damage mechanics, as an evolution equation that depends on the magnitude of local stress. In response to accumulated microdamage, osteocyte number density was modeled as a monotonically decreasing function of the microdamage, expressing osteocytic apoptosis due to microdamage. We hypothesized that the production of receptor activator of nuclear factor-κB ligand (RANKL), a master regulator of osteoclast differentiation, is triggered by osteocyte apoptosis and that RANKL production increases as osteocyte density decreases. In addition, the accumulation of microdamage leads to matrix degradation, which is expressed by a decrease in the elastic modulus of the matrix. Targeted remodeling for a single trabecula and a cancellous bone under uniaxial compressive loadings was simulated, in which the cancellous model was constructed from X-ray μCT data of a mouse femur. Under compressive loading, microdamage locally accumulated according to local trabecular morphology and mechanical conditions, and the corresponding regions were targeted to promote bone resorption by osteoclasts and subsequent new bone formation by osteoblasts. Thus, targeted remodeling under the influence of mechanics was reproduced in silico. The developed simulation method of targeted remodeling will be used as an in-silico experimental tool to investigate the coupled behaviors of mechanical adaptation and damage repair processes by bone remodeling. This study was supported by JST-CREST (JPMJCR22L5) and JSPS KAKENHI (JP20H00659, JP22K03827), Japan. We also thank Koki Fujimoto for technical assistance.

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EMPIRICALLY MODELING IONOSPHERIC ELECTRON DENSITY VARIATIONS USING F107 , E107 AND MGII INDICES BASED ON SCATTER RADAR OBSERVATIONS OVER LAGOS, NIGERIA.

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ABSTRACT

Each of three solar flux indices, F107 , E107 , and MgII core-to-wing, has been tested as asolar activity proxy to model empirically electron densityNe measurements made by anincoherent scatter radar during the period of 1976-2001 over the height span of 150-1000km at Lagos, Nigeria. It is found that deviations of model values given by the three indices to the data are practically the same, regardless of altitude, local time, and season,indicating no significant improvements with introducing the newer indices E107 and MgII for empirically modeling long-term Ne data. The long-term behavior of the three indicesare identical. This paper also discusses electron density responses to the solar flux index.

Computational mechanics in high-strain rate and impact engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT OF DRONE SUBSTITUTE MODEL FOR SURVIVABILITY ANALYSIS OF COLLISION WITH HUMAN HEAD

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ABSTRACT

A collision between drones and human head can have fatal consequences [1]. Considering that the dynamic response of two colliding solids depends on unknown impact conditions, geometry and material properties of each solid, the analysis of these risks turns out to be a very complex problem. The presented research idea is to develop a method derived from data science and AI augmented by physics, to help in the design of future drones (250g-4kg category). The approach proposed here is developed within the theoretical framework of mechanical wave propagation, that considers transient impact loading, contact duration, solid deformation and energy distribution within system. It considers the possible extension of the intrinsic properties of specific solid impedances [2], to more complex situations (multi-body and multi-material impactors, non-linear and dissipative phenomena, rupture) than usual. Simplified UAVs FE models, nevertheless based on shock physics, are used to access quantities relating to potential survivability on impact (forces, accelerations, transmitted energies), as functions of numerous simulation parameters, results which are analysed in relation to survivability envelopes, and reported to generalized design parameters like head/drone impedances.

The research first consists in carrying out numerical analyses to assess the physical basis and possible limits of the modelling proposal, as increasingly complex systems are studied. The contact force, momentum and energy transmitted during collisions between multi-material solids are evaluated (based on ONERA tests or open literature results [3]) and related to specific generalized impedances of impactors and targets. Once the FE substitution models (multi-domain, multi-material) for UAVs have been simplified (human head FE models are studied by an academic partner), the following work consists in carrying out a broad parametric numerical design of experiment (drone, velocity, impact angle, etc.) and in positioning the numerical results/data relatively to the prescribed survivability envelopes. The final stage of the research (perspective of the research) will concern AI-based data processing and comparison between raw (latent) and physically-based analyses.

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Machine learning and data driven based engineering computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MACHINE LEARNING HYPERPARAMETERS OPTIMIZATION FOR ENGINEERING PROBLEMS

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ABSTRACT

The flexibility of neural networks is also one of their main disadvantages as there are many hyperparameters to adjust in order to have an efficient architecture. For example, starting from an imaginable network configuration, one can change the number of layers, the number of neurons, the type of activation function to be used in each layer, the type of optimizer to be used, its learning rate, lot size and more (Géron 2023). Therefore, hyperparameter optimization is an effective process in building deep learning models as it consists of finding a good combination of these parameters to improve the model's performance. Exhaustive search and optimization tools are the strategies commonly used to obtain these best parameters. In this context, an initial alternative here was to use the Python Keras Tuner library. Specifically, this library helps with hyperparameter optimization for deep learning models built with TensorFlow and Keras (Géron 2023). When using optimizers, it is necessary to define, in addition to the objective function, to be minimized or maximized, the design variables and constraints. In the hyperparameter optimization problem, these are the design variables of the problem, the objective function is a metric that depends on the problem (classification or regression) and the constraints are of the variable limit type. This falls into a mixed variable optimization problem as it presents more than one type of design variable (integer and continuous). To achieve this, specific algorithms and strategies are needed to solve a problem of this nature. Still in the context of using optimizers to obtain hyperparameters, we investigated the following frameworks here: pymoo (Blank and Deb 2020), Optuna (Akiba, et al. 2019) and Ray Tune (Liaw, et al. 2018). These libraries offer a series of optimization algorithms, as well as tools to evaluate the performance of different algorithms on different problems. Initially, the Fashion-MNIST benchmark presented in (Géron 2023) with some techniques for obtaining the hyperparameters was studied. The frameworks explored here were then applied for an oil reservoir management problem. Results obtained by different frameworks are discussed.

Modeling and simulation of advanced manufacturing processes for metals
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MESHFREE COMPUTATIONAL MODELS OF METAL MANUFACTURING PROCESSES: THE GOOD, THE BAD, AND THE REAL WORLD

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ABSTRACT

Meshfree discretization methods have emerged as a powerful tool in computational mechanics, particularly in the context of manufacturing and materials processing simulations. The unique suitability of these techniques for multi-scale and multi-physics simulations stems from their efficiency in coupling different physical phenomena in a Lagrangian form and their inherent potential for adaptivity and parallelization, among other advantages. In this work, we present an overview of our recent developments in numerical simulations of various metal manufacturing processes using meshfree methods, with a focus on smoothed particle hydrodynamics (SPH). We examine the capabilities and limitations of our in-house massively parallel SPH code through a series of applications in both subtractive and additive manufacturing domains – see [1-3].

Computational modeling of manufacturing processes without mesh constraints offers attractive opportunities for developing multi-scale simulation approaches that can achieve remarkable efficiency. We demonstrate the ability of SPH to capture detailed thermo-mechanical aspects of metal machining operations, offering valuable insights into understanding processes, optimizing them, and controlling mechanisms. To achieve meaningful SPH simulation results, we emphasize the vital role of numerical stabilization and higher-order corrective terms through comparisons with experimental observations.

Furthermore, we showcase the strength and effectiveness of meshfree discretization techniques in representing the intricate fluid flow and melt pool behavior in metal additive manufacturing processes, such as laser powder bed fusion and cold spray 3D printing. We underscore the critical importance of runtime acceleration for manufacturing process simulation with SPH, highlighting the pivotal role of adaptivity and parallel computing in obtaining reliable numerical predictions.

This research offers a comprehensive examination of the potential benefits and challenges associated with employing meshfree methods, particularly SPH, in simulating metal manufacturing processes. By bridging the gap between theoretical modeling and real-world applications, our work not only lays the foundation for comprehending the key obstacles preventing widespread industrial adoption of meshfree methods but also suggests the necessary steps to take towards exploiting the full potential of these methods in multi-scale and multi-physics manufacturing simulations.

[1] https://doi.org/10.1016/j.apm.2021.08.010
[2] https://doi.org/10.1016/j.camwa.2023.03.003
[3] https://doi.org/10.1016/j.ijheatmasstransfer.2023.124378

ENHANCING CARDIOVASCULAR CFD SIMULATIONS WITH REDUCED ORDER MODELS

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ABSTRACT

Cardiovascular diseases, being major contributors to global mortality, present complex diagnostic and therapeutic challenges, making high-fidelity modeling techniques like Full Order Models (FOMs) essential for detailed hemodynamic analysis. However, the computational demands of FOMs, often built on finite element [1] or finite volume methods, limit their real-time clinical application. The emergence of digital twins as virtual replicas of a patient's cardiovascular system offers a groundbreaking tool in personalized healthcare, facilitating real-time diagnosis, treatment planning, and long-term health monitoring. Within this framework, Reduced Order Models (ROMs) emerge as a strategic solution, providing a streamlined yet accurate representation of these complex models, enhancing computational efficiency without significant loss of critical details.

In this presentation, we will explore how ROMs complement FOMs, creating a more versatile and practical approach to cardiovascular CFD. We will discuss the potential brought by two different approaches, namely traditional intrusive physics-based ROMs and data-driven techniques (particularly those based on machine learning and neural networks), in enhancing the predictive capabilities of these models. This is crucial for developing adaptive models suitable for the variability and complexity of cardiovascular conditions in clinical settings.

A key part of this presentation will be the introduction of a test case for multi-scale hybrid ROM simulations for cardiovascular flows [2]. This case study addresses the challenge of enforcing patient-specific non-homogeneous Dirichlet boundary conditions on pressure within an intrusive ROM framework, employing a lifting function approach. We utilize the Finite Volume (FV) method for simulating multi-scale blood flow in idealized or realistic cardiovascular geometries. The talk will compare two stabilization techniques: one based on supremizers and the other on the Pressure Poisson Equation. Our objective is to enable the incorporation of time-dependent boundary conditions for both velocity and pressure at the reduced level, potentially enhancing the accuracy and efficiency of cardiovascular simulations. This development could lead to more realistic and patient-specific modeling in cardiovascular care.

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Recent advances in numerical methods for mixed-dimensional PDEs
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TDC FOR FINITE ELASTIC DEFORMATION IN SUBMERGED MOORING LINES EXPOSED TO DYNAMIC LOADING

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ABSTRACT

The next generation of offshore and nearshore structures will be focused towards expanding human activities into the ocean waters. These range from power generation using floating solar platforms, aquaculture farms and floating islands for use in farming, housing and production facilities. These structures are expected to have a large waterplane area and a structurally compliant design to enable them to survive the harsh offshore environment. Moreover, these platforms are also expected to require new mooring methods involving flexible synthetic mooring lines, especially for deployment in relatively shallow waters.

These problems require development of models capable of effectively capturing the geometric nonlinearity in the structural deformation associated with large deformations of flexible bodies. In these cases, the equilibrium is satisfied in the deformed configuration, while the problem is often formulated in the presently known undeformed configuration, resulting in a moving boundary problem. Moreover, modelling of structures like mooring lines involve dimensional reduction over curved manifolds, resulting in considerably more involved partial differential equations.

In this work we present a finite-element model for flexible mooring lines, capable of capturing the geometric nonlinearity associated with large deformations. We utilize the Tangential Different Calculus (TDC) method, devised in Fries (2020), for defining the geometric and differential quantities associated with finite strain (large deformation) analysis of mooring lines over curved manifolds. The technique can be applied on parametric and immersed manifolds, thus enabling the application to embedded flexible boundaries. However, this work will present the results only using the parametric manifold approach. The effect of the sea-floor is implemented using a damped spring bed, thus enabling large movement of the touch-down point of the mooring line. Additionally, the effect of the wave and current loading on the mooring line is implemented using Morison’s equation, with slender body approximation. The model is implemented using Gridap (Badia 2020), an advanced FEM library in Julia language. We utilize this model to study the variation in the tension at the fairlead and the anchor of a composite mooring line, comprised of chain and fiber sections, under wave and current loading. The work will highlight the influence of geometric nonlinearity on the tension and the excursion of the floater.

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Current trends and advances in enriched finite element methods and coupled simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ACCELERATING FRACTURE MECHANICS SIMULATIONS THROUGH MODEL ORDER REDUCTION WITH ENRICHED REDUCTION SPACES

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ABSTRACT

This work introduces a model order reduction method for accelerating the solution of fracture mechanics problems, discretised with enriched finite elements. Projection based approaches, which are the most common among model order reduction methods, rely on the assumption that solutions of high dimensional problems can be accurately approximated in low dimensional spaces, that can typically be obtained from solutions to similar problems. In fracture mechanics problems however, the presence of evolving localised discontinuities, in the form of cracks, significantly limits the effectiveness of such bases. As a result, most existing model order reduction methods for such problems are either limited with respect to the damage configurations that can be represented or require frequent solutions of the full order problem to update the low dimensional spaces used, in order to account for crack propagation, thus reducing efficiency. In the proposed approach, low-dimensional spaces, constructed for undamaged systems, are adaptively enriched with selected columns of the flexibility matrix of the system, allowing to represent arbitrary crack configurations. It is shown that the resulting spaces contain the solution to the full problem, while their dimension is significantly reduced. However, to render the online construction of such spaces efficient for general crack configurations, the full inversion of the initial system’s stiffness matrix is necessary, a task that is computationally infeasible. To lift this limitation, hierarchical matrix representations are used, which significantly reduce the complexity of this operation by representing matrices in a data-sparse format. The resulting method achieves significant computational gains, without sacrificing the flexibility and accuracy of the full-order model. The performance of the approach is demonstrated through examples involving cohesive crack propagation.

Multiphysics and data-driven modeling for cardiovascular biomedicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EVALUATION OF PHYSICS-INFORMED NEURAL NETWORKS PERFORMANCE FOR AORTIC BLOOD FLOW SIMULATION UNDER DIFFERENT SEVERITY OF STENOSIS

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ABSTRACT

Background:
Physics-informed neural networks (PINNs) have emerged as a powerful approach to encode governing PDEs and training data to inversely model complex engineering problems. Recent efforts have aimed to solve the Navier-Stokes equations with applications to vascular blood flow. However, key limitations inherent to neural networks, such as spectral bias, which tends to bias the training to low-frequency functions can notably reduce solution accuracy. Since cardiovascular flows can become transitional or quasi-turbulent, spectral bias can exacerbate the errors. To address this challenge, we have developed a PINNs architecture that uses a Fourier-based activation function, borrowed from computer vision literature, and investigated the accuracy of our Fourier-based PINNs architecture under a range of patient-specific blood flow conditions.

Methods:
CFD Simulations: Aortic geometry was obtained from the open-source repository (www.vascularmodel.com, patient ID: 01750000). The geometry was deformed to virtually induce a stenosis severity of 0 - 70% in increments of 5% (N=15 cases). High-resolution CFD simulations (mesh size = 7M elements, # timesteps=10,000) were performed. Inlet Reynolds number was 823 while local Reynolds number in the stenosis ranged from ~600 – 2000. Sensor points were randomly sampled at 1600 points.
PINNs Architecture: The solution to the velocity field was approximated using a fully connected neural network, which is a function of spatial coordinates, time and network parameters. Three loss function were used in the optimization process to further regularize the solution: i) losses from the Navier-Stokes equation; ii) losses from the partially-known boundary conditions; and iii) losses from the known sensor data. Adaptive coefficients were used to control the weighting of these loss function during the training process. Skip connections were used to further improve the accuracy and minimize vanishing gradients. Sinusoidal activation functions were used due to their ability to represent high-frequencies in the data. Swish and Tanh activation functions were also used for comparison.

Results and Conclusion:
L2-Norms ranged from 0.63 to 0.3 and absolute percent error ranged from 45% to 19% from lowest to high stenosis severity. Sinusoidal activation function had an accuracy that was 13% and 12% higher compared to swish and tanh for the highest stenosis severity (i.e., 70%). Our findings demonstrate that while under laminar blood flow conditions, PINNs errors may be within reasonable range of ~15%; however, in transitional or quasi-turbulent flow conditions, the errors

can increase drastically. Further work should focus on fundamental improvements in PINNs for modeling complex transitional blood flow conditions.

Emerging topology and shape optimization techniques in computational design of materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LEVEL SET TOPOLOGY OPTIMIZATION FOR THE DESIGN OF ELASTIC SHELL SOLIDS

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ABSTRACT

The goal of the project is to develop a topology optimization framework for the design of elastic shell structures. Shells are three-dimensional solid structural elements whose thickness is slender compared to its other dimensions, which makes them highly desirable across several fields of engineering for their structural efficiency. Current simulation tools have become prevalent to assist their characterization, however they are still elusive in providing optimized geometric solutions that comply to the requirements and constraints imposed by the shell geometry. In this work, we combine the Reissner-Mindlin kinematics and the level set method to systematically capture the optimal hole placement within a background shell mid-surface. For a given set of load cases and constraints, we synthesize the best three-dimensional surface shape that minimizes a functional, either compliance and/or stress under a volume constraint. A sensitivity analysis, combining the Hadamard shape derivative and the topological gradient, is conducted in curvilinear coordinate system. For the stress measure, the p-norm function is employed to integrate stress fields into a global stress measure. To the reduce the sensitivity with respect to the starting shape in the algorithm, we make use of the reaction-diffusion approach to update the level set function. To this end, the optimization problem is regularized by introducing fictitious interface energy, which acts as a perimeter minimization constraint. With this method, the desired number and shape of the holes can be tailored adjusting the value of the diffusion coefficient.
The efficiency of the method is compared to an equivalent three-dimensional solid optimization problem, executed under similar conditions on structures of thin-walled geometry. We design several shell structures of increasing complexity, from continuous by part flat plates, to curved surfaces, manifolds and non-manifolds with creases. Each example requires 250 iterations maximum to converge, which take about 10 min on a machine with 12 CPU. In most examples, the last hole nucleation or vanishing occurs around iteration 100, the last iterations only contributing to minor improvements. The obtained geometries are highly regular and compliant with respect to cutting processes. In comparison, the exact same algorithm applied to three-dimensional solid elements takes several hours to accomplish the same number of iterations, yielding a similar outcome, with slightly improved performances, but with an organic aspect (Fig. 1). Finally, the level set description enables to rapidly extract the surface which can be converted into B-Rep and used subsequently in CAD and CAM software.

Multi-scale, multi-rate damage and fracture: Models, experiments, and simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MOVING WINDOW CONCURRENT ATOMISTIC CONTINUUM APPROACH FOR MODELING SHOCK WAVE PROPAGATION IN MULTIPLE PRINCIPAL ELEMENT ALLOYS

Alexander Davis[1], Abigail Hunter[2], Saryu Fensin[2] and Vinamra Agrawal[1]*

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ABSTRACT

Spall fracture is one of the most common ways a material can fail under high-strain rate loading. Extensive experimental investigations have indicated that microstructural features such as grain boundaries play a crucial role in the nucleation of voids leading to spall fracture. In this work, we develop a novel moving window concurrent atomistic continuum (MW-CAC) model to study shock propagation in face-centered cubic single-component (Cu) materials and multicomponent (FeNiCr) alloys. The technique uses the concurrent atomistic continuum (CAC) method that uses the unified formulation obtained from the Atomic Field Theory.

We study a Riemann problem involving a planar shock in a 3D domain with constant states (strain, particle velocity, temperature). We use the atomic resolution at the shock wave and continuum resolution outside. We track the moving shock wave using two moving-window algorithms - the conveyor and coarse-refine methods. In the conveyor method, we add and remove planes of atoms at regular intervals to recenter the moving shock in the atomistic window. In the coarse-refine method, we refine (coarsen) the continuum elements ahead (behind) the shock to follow the moving shock wave and keep it centered in the atomistic window. Next, we use the A-atom approach to introduce average atoms for simulations involving multiple principal element alloys. We use the A-atoms in the continuum regions. We study shock propagation in Cu and FeNiCr alloys with two equations of state (EOS), the linear Hugoniot and the thermoelastic Eulerian equation. We study shock front thickness and planarity as it evolves. The MW-CAC approach demonstrates excellent speed-up compared to large-scale non-equilibrium molecular dynamics simulations

Multi-physics and multi-scale simulations with the coupling library preCICE
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ASSESSMENT OF FLOW-INDUCED STRESSES IN SPIRAL WELD PIPES WITH BENDS

Shahab Ahmadizade[*1], Suyash Verma[1] and Arman Hemmati[1]*

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ABSTRACT

This study focuses on the computational modeling of fluid-induced stresses and their effects on curved spiral-welded liquid pipelines. We employ two distinct open-source solvers with different computational approaches to address the fluid-structure interaction (FSI) problem. First, Solids4Foam is utilized for the complex FSI analysis, which is an internal component of OpenFOAM. The second solver is CalculiX, a separate open-source tool for finite element analysis (FEA), notable for its compatibility and integrative potential with OpenFOAM. Our parameter space follows the operating dataset of two major pipeline industry leaders, which includes the design and material information of their liquid pipelines. Our study specifically targets pipelines with varying bend angles and radii under regular and fatigue conditions. These scenarios are initially simulated using unsteady Reynolds-Averaged Navier-Stokes (RANS) models, incorporating the k-ω turbulence model in OpenFOAM. After the initial assessment of the flow dynamics and development of our first stress-prediction model, we upgrade our fluid modeling technique to Detached Delayed Eddy Simulations (DDES), which combines the high-accuracy Large Eddy Simulation (LES) formulations with k-ω RANS model.

For this conference, we will focus our attention on challenges and limitations of FSI analysis with available techniques, particularly solids4Foam. Solids4Foam is sensitive to how meshes conform when transferring data between fluid and solid domains. If meshes on the solid and fluid components are not properly aligned in size and conformity, Solids4Foam encountered challenges in adjusting the criteria for simulation convergence. The application of certain boundary conditions, particularly contact boundary conditions in the solid domain, presents complexities and may restrict the scope of the simulation. This limitation also complicated using varied materials within the solid domains, thereby further reducing simulations' flexibility. To address these limitations, we integrated preCICE and Calculix with OpenFoam. This strategy is designed to allow handling of more complex scenarios within the solid domain, thus offering a robust solution for fluid-structure interaction simulations. By utilizing these tools, we have improved both the accuracy and efficiency of our analysis, ultimately contributing to the enhancement of pipeline system design and structural integrity. This research represents a significant step forward in our understanding of fluid-induced stress prediction and assessment in pipelines. The ultimate objective of this work is development and deployment of a software package that utilizes reinforced learning, based on simulation and experimental data, to predict the formation and propagation of cracks induced by flow-induced stresses in pipelines at various operating conditions.

Mathematics and algorithms for predictive digital twins (DT)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTIFIDELITY OPERATOR NETWORKS FOR CLOSURE MODELING IN MULTISCALE SYSTEMS

Shady Ahmed[*1] and Panos Stinis*[1]

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ABSTRACT

Digital twin applications require a synergy between the physical system and its virtual counterpart. In a typical application, the computational model is queried multiple times during the operation of the system where quick responses are necessary to monitor, control, and optimize the performance of the physical asset. Traditional simulation techniques are often too computationally expensive that they fail to fulfill the tight turnaround time requirements. Therefore, computationally-lightweight models are essential components of digital twin frameworks.

The trade-off between accuracy and cost can be addressed by identifying the key features and coherent structures of the system and building reduced order models to capture the dynamics of these large-scale phenomena. However, for multiscale systems, these models usually suffer in long time predictions due to the rapid propagation of errors in the small scales to contaminate the simulation of large scales. Closure modeling refers to correcting reduced order models' predictions by accounting for the effect of the truncated scales on the resolved ones. We look at the closure problem from a multifidelity learning perspective. In particular, a combination of proper orthogonal decomposition and Galerkin methods is used as the low-fidelity dynamical model for the dominant modes. Meanwhile, deep operator networks are utilized to make up for the contribution of the small scales in a multifidelity setup. Numerical experiments are carried out using prototypical benchmarks representative of large-scale geophysical flows prevalent in digital twins of Earth systems. Results show that operator networks can learn correction terms across a wide range of initial conditions and parameter values with reliable predictions for long forecast lead times.

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Minisymposium in honor of Prof. Yannis Kallinderis's 60th birthday: Progress of Unstructured grid based CFD, hybrid mesh generation and adaptation, and parallel supercomputing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATION OF UNSTRUCTURED GRID-BASED CFD SIMULATIONS IN NAVAL AND SHIP HYDRODYNAMICS

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ABSTRACT

The unstructured grid technique, pioneered by researchers such as Mavriplis, Nakahashi, Luo, Lohner, and Kallinderis[1] since the early 1990s, has primarily been employed in aeronautical applications. However, there is a growing trend to extend these technologies to the field of ship and naval hydrodynamics. This presentation will focus on the utilization of unstructured grid CFD simulation technologies in ship hydrodynamic applications[2]. Various challenges unique to ship hydrodynamics will be addressed, and potential solutions[3] will be discussed.

[1] Strongly coupled flow/structure interactions with a geometrically conservative ALE scheme on general hybrid meshes
HT Ahn, Y Kallinderis; Journal of Computational Physics 219 (2), 671-696

[2] Incompressible Navier–Stokes method with general hybrid meshes
Y Kallinderis, HT Ahn; Journal of Computational physics 210 (1), 75-108

[3] Hyperbolic cell-centered finite volume method for steady incompressible Navier-Stokes equations on unstructured grids
HT Ahn; Computers & Fluids 200, 104434

Quantum scientific computing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

QUANTUM ANNEALING FOR PARTICLE MATCHING IN QUASI-CYCLIC DISCRETE-ELEMENT METHOD SIMULATIONS

Oliver Ahrend[*1] and Julia Kowalski*[1]

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ABSTRACT

There is an increasing interest in utilizing the potential of quantum computing for a wide range of compute-intense tasks across many academic and industrial disciplines. Different quantum computing technologies have been proposed that today are available in maturity levels ranging from the mere existence of a conceptual idea to ready-to-use technologies. So-called quantum annealers (QAs) are an example of the latter and exploit quantum fluctuations to solve special classes of discrete optimization problems. Today's QAs have many times more qubits than gate-based quantum computers, and can be used to study realistic problems. Here, we feature an engineering application, in which a particle matching algorithm arising in a quasi-cyclic discrete element method simulation is reformulated for a QA as a QUBO model. Implementation on a QA (D-Wave), however, requires us to select a large number of hyperparameters, such as annealing time, readout thermalization, programming thermalization. Based on the observation that typically the probability of sampling a correct solution is very low and large problems can not be solved reliably, a systematic sensitivity analysis would be desirable. So far, however, literature mostly provides information on the sensitivity in single parameters [1, 2, 3]. In this contribution we will address this lack of information. We first describe how a particle matching task can be reformulated for a QA, and show how a run is conducted. We then summarize the different types of hyperparameters present in the algorithm. Next, a sensitivity study is conducted to identify and analyze the correlation between solver parameters and parameter of the problem setting. We discuss our results and conclude on parameter selection strategies that guarantee a reliable solution.

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Multiphase flow and non-Newtonian fluid - Modelling and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DYNAMICS OF BUOYANT MISCIBLE INJECTION FLOWS IN A CONFINED MEDIUM

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ABSTRACT

In this study, we investigate buoyant miscible injection flows of a high-dense fluid into an inclined closed-end pipe filled with a low-dense fluid. We use mainly experiments, accompanied by complementary numerical simulations and semi-analytical methods, to analyze the influences of the flow and fluid parameters on the flow dynamics. The fluids are miscible, and the timescale of our experiments is adequately short so that the fluids do not mix remarkably. To generalize the results, the relevant dimensionless numbers of the flow are used, including the Froude number (Fr), the Reynolds number (Re), the buoyancy number (χ), the Archimedes number (Ar), the viscosity ratio (M), the Bingham number (B), the inclination angle (β), the aspect ratio (δ), the radius ratio (Rc), and the eccentricity (E). Results show that for the injection of a high viscous fluid, the separation of the heavy fluid front from the bulk of the fluid happens when Re and β are large [1]. For the injection of a viscoplastic fluid, a core fluid immersed in the in-place fluid is formed, for which there appear three different flow patterns, namely, the breakup, coiling, and bulging regimes [2,3]. In the breakup regime, as the injection continues and time grows, the injected viscoplastic fluid can no longer withstand the progressively-increasing buoyancy force, causing the yielding of the core fluid towards thinning and, ultimately, the core breaks up. In the bulging regime, the pressure and the interfacial shear stress applied by the upward flow of the in-place fluid on the core lead to yielding towards the bulging of the core. For the coiling regime, the core fluid remains unyielded and its diameter is unchanged until it distorts into a coiling structure. We develop a lubrication approximation model using the Herschel-Bulkley constitutive equation. Based on a rational prediction of the onset of yielding, we can classify the flow regimes versus an elegant combination of the dimensionless flow parameters, including B, χ, M, and δ.

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Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

3D PRINTED ARCHITECTED SHELL-BASED FERROELECTRIC METAMATERIALS

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ABSTRACT

Ferroelectricity allows the generation of electrical power from mechanical oscillations and temperature fluctuations. Tailoring the underlying microarchitecture of ferroelectric materials imparts a promising route for enhancing their ferroelectric performance. In this study, we resort to shell-based architected materials to construct ferroelectric metamaterials with controllable multiphysical properties. A modified multiscale simulation, incorporating the poling process of architected piezoelectric materials, is developed to accurately determine their effective electromechanical properties. The interplay among relative density, shell topology, and ferroelectric figures of merit, metrices for assessing the performance of ferroelectric metamaterials as sensors and energy harvesters, is explored. A high-resolution 3D printing technique is adopted to fabricate the architected piezoelectric metamaterials; experimental measurements of their piezoelectric charge and dielectric constants corroborate their excellent sensing and energy harvesting functionalities in the next generation of lightweight intelligent infrastructures.

Model order reduction for parametrized continuum mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODEL-BASED DESIGN APPROACH FINDING OPTIMAL LIQUID COOLING FLOW PATH FOR ELECTRIC VEHICLE BATTERY

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ABSTRACT

In the early products of electric vehicles (EV), an air-cooling method was employed for the battery thermal management system (BTMS), however, because of more severe heat generation, many EV companies have adopted liquid cooling methods for more efficient cooling. BTMS shape is usually plate-like structure on box shaped batteries. In these BTMS, it is a critical determinant for thermal performance where are flow paths in their plates. If we can estimate these performances and design flow paths in early product development phase, it facilitates subsequent development process. For estimating such industrial thermal flow problems, Computational Fluid Dynamics (CFD) is assumed an important role. However, in early product development phase there are sometimes many shapes (results of trial-and-error), so it is difficult to simulate them all for CFD calculation cost. We study how to solve these issues based on Model based design and Machine learning. At first, for simplicity, we defined that these flow paths can be expressed in the form of graph data. These plates are discretized into elemental components as nodes with connections represented as edges. Next, we solve the equations of conservation of mass, pressure loss, and conservation of heat which are given by the relationships between nodes and edges. The coefficients of these equations are defined with each shape feature and adjusted to fit CFD results in advance, so this simulation methods results are like CFD ones. In this paper, we introduce the simulation and examples of shape parametric optimization to demonstrate the advantage of the proposed approach in terms of speed and simulation cost.

SciML in the real world
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

OPTIMIZING GRADIENT BACK-PROPAGATION FOR HYBRID NEURAL DIFFERENTIABLE SOLVERS

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ABSTRACT

Hybrid neural differentiable models represent a significant advancement in scientific machine learning, standing on the innovative concept of seamlessly integrating domain-specific knowledge with cutting-edge deep learning models, offering a novel solution to the limitations of both traditional numerical solvers and neural networks. Traditional models are effective for well-understood physical phenomena but struggle with complex systems, while neural networks excel in learning unknown/unresolved physics from data but often lack in interpretability and can have difficulties in generalizing to new situations. By combining these approaches, hybrid models aim to leverage the advantages of both, leading to improved predictive capabilities in modeling complex physical systems and potentially discovering new physics from sparse and indirect data.

The effectiveness of these hybrid models depends largely on the differentiability of the solvers they use. Differentiable programming addresses this need, allowing for the joint optimization of machine learning and numerical model components within a unified framework. This field has seen growing interest, with differentiable solvers and hybrid models showing potential in a variety of scientific applications. However, training these models can be challenging, particularly when dealing with dynamic data over long timeframes or when using iterative solvers, such as implicit or Poisson solvers. These situations can create extensive computational graphs for gradient calculations, leading to high memory requirements and concerns about the scalability of the models. This research will investigate methods for effectively training hybrid neural differentiable models, particularly in scenarios involving long-term model rollout or iterative implicit learning scenarios. The evaluation will center on the effectiveness of these methods in decreasing computational requirements, while also addressing the possible drawbacks associated with these techniques.

Machine learning for large scale models in physics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A CONSISTENT NON-LINEAR AND GEOMETRICAL REDUCED ORDER MODELING APPROACH WITH UNCERTAINTY QUANTIFICATION APPLIED TO THE CONVECTION DOMINATED INCOMPRESSIBLE NAVIER-STOKES EQUATIONS

Nissrine Akkari[1] and Fabien Casenave*[1]

[1]*Safran*

ABSTRACT

In this work, we propose a non-linear and geometrical Reduced Order Model ROM using a Gaussian Mixture Variational AutoEncoder (GMVAE) [1]. GMVAEs are proposed in the literature for unsupervised data clustering using Gaussian Mixture Models (GMMs).

In the offline stage, the GMVAE compresses the instantaneous velocity and pressure fields of the fluid flow of a variable geometry, along with the fields describing the masks of the geometries respectively for each unsteady solution at a given geometric configuration.

In the online stage, unlike the least-square minimization of the ROM residual [2], the zero-constraint of the residual enables uncertainty quantification by sampling from a specific statistical model from the learned mixture of statistical models. In fact, the geometrical reduced order model coefficients are obtained by solving the zero-constraint of the residual of the Navier-Stokes equations, which is based on the non-linear projection of the residual upon the latent space of the GMVAE using the encoder part of it. A consistent formulation of this reduced order model is guaranteed thanks to the encoding of a time discretization of the velocity term in the Navier-Stokes equations [3]. The geometrical reduced order solution at a given time instant and at a given geometry of the fluid flow is obtained thanks to the decoding of a sample of a statistical model from the mixture latent features. This statistical model is inferred by encoding the terms of the Chorin predictive and corrective scheme at the preceding time step and, the mask of the current geometry.

The proposed geometrical and unsteady non-linear reduced order model is applied to the convection dominated incompressible Navier-Stokes equations, in order to infer the unsteady and turbulent flow past a NACA2412 generation at an angle of attack equal to 30°, with a variable thickness and chord length.

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MECHANICAL BEHAVIOUR OF TUBULAR TOPOLOGICAL INTERLOCKING ASSEMBLIES

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ABSTRACT

A topological interlocking assembly is an arrangement of several rigid blocks that are in contact with each other and are constrained by a fixed frame such that each subset of blocks is kinematically constrained and therefore cannot be removed from the whole assembly. The platonic solids are examples of convex blocks that allow such interlocking assemblies, see [1]. Exploiting topological interlocking enables the construction of large concrete structures without the usage of mortar as binding material. Over the years various blocks that give rise to topological interlocking assemblies by assembling copies of a given block, have been proposed. Dyskin et al. are notable pioneers in the field of topological interlocking [1]. In [2], the authors provide an recent overview of assemblies with interlocking properties.

In this presentation, we discuss an algebraic construction method that facilitates the design of various topological interlocking assemblies. More precisely, we construct blocks whose copies can be assembled to form tubular structures with interlocking properties. This is achieved by exploiting two dimensional crystallographic groups, i.e. the symmetries of periodic wall paper patterns. Here, we focus on the design of tubular topological interlocking assemblies that prevent certain simultaneous movements of the blocks in the assembly when the frame remains unfixed. The motions of interest are the simultaneous radially outwards movement of every block. Hence, we generate examples of tubular interlocking assemblies that prevent the described motions and compare their structural behaviour to the behaviour of interlocking assemblies that do not prevent these movements when the frame is not fixed. In particular, we achieve this comparison by conducting several finite element studies. Moreover, we address the challenge of manufacturing the proposed structures with carbon
reinforced concrete.

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Enabling technologies for digital twins: Model reduction and scientific machine learning
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INCREMENTAL TENSOR DECOMPOSITIONS FOR BUILDING EFFICIENT DIGITAL TWINS

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ABSTRACT

With recent advancements in large-scale parallel computing, there is an increased interest in constructing high-fidelity digital twins of complex systems. Especially for systems that have limited physical experimentation possibilities, high-fidelity simulations may provide the main source of information for constructing digital twins for deployment into online operations. However, performing such simulations is computationally intensive and generates extreme amounts of data. The size of the generated simulation data makes it challenging to use the data in further analysis. As the spatial and temporal resolution of these simulations grow, even storing the data may become a serious bottleneck.

In this talk we address this problem through the use of low-rank tensor decompositions. Specifically, we will present incremental algorithms that provide computationally efficient ways of compressing generated data with accuracy guarantees. We demonstrate the efficacy of incremental tensor decompositions through tensor train and hierarchical Tucker formats. Our research presents two specific algorithms: The Tensor Train Incremental Core Expansion (TT-ICE)[1], an incremental tensor train decomposition algorithm that offers state of the art compression speed, and Hierarchical Incremental Tucker (HIT)[2], the first known algorithm in the literature to perform incremental updates to hierarchical Tucker format.

Beyond the advantage of space savings, our algorithms offer a reduced representation that facilitates downstream learning tasks such as Bayesian inference and deep learning[3]. Our results reveal computational savings concerning memory requirements and execution time for the incremental algorithms compared to their traditional one-shot counterparts. We validate our findings using datasets from parametric-PDE-driven simulations of a chaotic system and particle-in-cell simulations of an electric propulsion system. Those examples demonstrate the scope of our approach's applicability.

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Emerging topology and shape optimization techniques in computational design of materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPLOITING RATE-DEPENDENT INSTABILITIES IN SOFT METAMATERIALS THROUGH SHAPE AND TOPOLOGY OPTIMIZATION

Ryan Alberdi[*1], Craig Hamel[1], Aabhas Singh[1], Kevin Long[1] and Adam Cook[1]*

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ABSTRACT

Soft metamaterials can offer programmable responses to external stimuli, making them desirable for applications such as soft robotics, shock and vibration mitigation, and flexible electronics. In line with the metamaterial concept, the response of these materials is governed to a large extent by the geometric and topological makeup of their small-scale features. However, the link between structure and response is less intuitive for soft metamaterials due to their reliance upon highly nonlinear instabilities. This is further complicated by the effects of viscoelastic relaxation, which recent studies have shown to alter the emergence of instabilities in non-intuitive ways. To exploit this complex design space and advance the development of soft metamaterials, we propose a computational design framework based on shape and topology optimization. Our software stack employs a unique library for solving nonlinear solid mechanics problems that poses them in an energy minimization form to robustly handle instabilities while accounting for the path-dependence of viscoelastic phenomena. Moreover, a modular architecture allows for the use of both CAD-parameterized shape optimization and level-set topology optimization. We present examples demonstrating how this approach can be used to tailor the rate-dependent response of soft metamaterials exhibiting snap-through and buckling instabilities.

Emerging topology and shape optimization techniques in computational design of materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

POLYPLAS: A PYTHON IMPLEMENTATION OF A TOPOLOGY OPTIMIZATION FRAMEWORK FOR PLASTICITY WITH UNSTRUCTURED POLYGONAL FINITE ELEMENTS

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ABSTRACT

We present PolyPlas, a Python program for a structural topology optimization framework considering von Mises plasticity with unstructured polygonal finite element meshes. The modular structure of this code is inspired by PolyTop, an educational code for compliance minimization for linear elastic material. Unlike the previous PolyTop program, PolyPlas is fully realized in Python for the purpose of open-source access to both academic and industry users alike. The nonlinear physics are modeled by the radial return mapping algorithm coupled with a displacement control subroutine. A discussion on volumetric locking effects in conjunction with the polygonal finite elements is also included herein. Finally, several numerical examples are presented to illustrate the capabilities and efficiency of PolyPlas in solving topology optimization problems considering von Mises plasticity.

Scientific deep learning
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTI-LEVEL NEURAL NETWORKS FOR ACCURATE SOLUTIONS OF INITIAL AND BOUNDARY-VALUE PROBLEMS

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ABSTRACT

In recent years, machine learning approaches, such as the physics-informed neural networks (PINNs)[1], the deep Ritz method[2], or the weak adversarial networks[3], have shown promising results for several classes of initial and boundary-value problems. However, their ability to surpass, particularly in terms of accuracy, classical discretization methods such as the finite element methods, remains a significant challenge. One of the main obstacles of deep learning approaches lies in their inability to consistently reduce the relative error in the computed solution. We present a novel approach, the multi-level neural networks, in order to reduce the solution error when using deep learning methods. The main idea consists in computing an initial approximation to the problem using a simple neural network and in estimating, in an iterative manner, a correction by solving the problem for the residual error with a new network of increasing complexity. This sequential reduction of the residual associated with the partial differential equation allows one to decrease the solution error, which, in some cases, can be reduced to machine precision. The underlying explanation is that the method is able to capture at each level smaller scales of the solution using a new network. Numerical examples in 1D and 2D dealing with linear and non-linear problems will be presented to demonstrate the effectiveness of the proposed approach.

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Advances in computational biomechanics and mechanobiology
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MODEL FOR STRAIN RATE DEPENDENT REVERSIBLE CYTOSKELETAL FAILURE IN CELLS EXPOSED TO SUPER-PHYSIOLOGICAL DEFORMATION RATES

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ABSTRACT

All cells are exposed to mechanical forces and deformations, and must be able to rapidly adapt to maintain their functional integrity. To better understand the relationship between applied loads and cellular mechanics, we have developed a method for directly measuring single-cell mechanical properties called cellular micro-biaxial stretching (CμBS), which uses traction force microscopy methods coupled with a device that applies precise deformation to the substrate on which the cells are seeded. We recently performed a series of experiments wherein we applied a repeated rapid stretch and hold deformation with varied stretch rate to micropatterned vascular smooth muscle cells. We found that, regardless of the rate at which the cells were stretched, all cells displayed stress-relaxation, typical of viscoelastic materials. But, increasing the stretch rate yielded decreased stresses, which directly conflicts with conventional viscoelastic models. In fact, cells exposed to super-physiological strain rates, mimicking trauma, displayed nearly no increase, and often a decrease, in stress following stretch. While these results suggest that some component of the cell is failing at high strain rates, repeated stretch experiments showed that in most cases the stress is recovered in subsequent stretches, so the observed decrease in stress is not due to plastic deformation. To explain this phenomenon, we have developed a model of stress fiber strain rate dependent reversible failure, in which actin-myosin binding kinetics are dependent on fiber stress and fiber stress is strain-rate dependent. Here, I will present this model and its implications for cellular mechano-adaptation.

16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Advancements in model reduction, data assimilation, and uncertainty quantification for complex physical systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A METHOD TO CONSTRUCT LOW RANK TENSOR NETWORK POLYNOMIAL REDUCED ORDER MODELS

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ABSTRACT

We present an efficient method to fit low-rank multivariate polynomials to implicitly defined smooth mappings between high-dimensional spaces. By implicitly defined, we mean that evaluating the mapping requires solving a large non-linear system of equations. Such mappings arise as, e.g., parameter-to-output mappings in inverse problems governed by partial differential equations (PDEs). To overcome the curse of dimensionality, we represent arrays of polynomial coefficients in low-rank Tucker-tensor-train format. Tucker-tensor-trains are fit to data generated by evaluating the mapping and, crucially, symmetric actions of high order derivatives of the mapping. Derivative actions are computed using adjoint-based techniques. We use the method to approximate key mappings in several PDE-based inverse problems. The results show that (1) it is feasible to construct high order (e.g., 6th order) polynomial reduced order models, and (2) using high order polynomials and derivatives substantially increases accuracy.

Smart structures – Modelling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FINITE ELEMENT MODELLING OF MATERIALLY UNIFORM DIELECTRIC ELASTOMERS

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ABSTRACT

Non-magnetisable electroelastic materials are characterised by a strong coupling between elastic and electrostatic properties. Dielectric elastomers are electroelastic materials that can undergo very large deformations when subjected to electric fields, and have attracted much attention due to the vast range of applications as sensors and actuators. The foundations for the study of this class of materials have been laid by the seminal works of Toupin [2] and several others. In brief, the Helmholtz' free energy is a function of both the deformation and the electric polarisation, so that both contribute to the stress.
We are interested in the theory of uniform elastic dielectric. In the theory of material uniformity established by Noll [1], a body is uniform if all points are made of the same material. When this is the case, there is an "archetypal" point from which all points can be mapped by means of a tensor field called implant tensor. The theory can model a vast range of inhomogeneous materials, i.e., materials for which the material properties depend on the material point. The case of homogeneous bodies is retrieved when the implant tensor is constant, i.e., independent of the material point. For an electroelastic body, uniformity implies that the Helmholtz' free energy depends on the material point exclusively through the implant tensor.
In this study, we developed a finite element solver in Matlab, designed to handle electromechanical simulations and whose capabilities are demonstrated by simulating a layered-beam-type actuator. The beam has two layers made of the same dielectric elastomer, with the top layer sandwiched between two (ideally) infinitely compliant electrodes, between which a difference of potential is applied. In this way, only the top layer of the beam is activated and thus the beam bends when actuated.
The inhomogeneity simulated in our test is contorted aeolotropy: the implant tensor is a randomly generated orthogonal tensor depending on the material point. In this way, the implant represents a particular case of local distortion. Under an applied electric field, the inhomogeneous beam not only bends but also warps, in contrast to a perfectly homogeneous beam. The study of inhomogeneities is important to predict potentially undesirable warping of this type of actuators. We plan to apply this model to other actuator geometries and loading conditions.

HYPEROPTIMIZATION INSIGHT FOR TOPOLOGY OPTIMIZATION

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ABSTRACT

The nonlinear relationship between the form and function of physical structures in our built environment raises challenges for design. Modern design methods, such as topology optimization, provide structural solutions but obscure the relationship between the form of the solution and the formulation of the underlying design problem. Here, we show how to extend classical molecular dynamics methods to provide novel forms of insight into the origin and organization of design features in problems typically studied via topology optimization. Our computational approach to morphogenesis problems extends topology optimization techniques by adapting physics-based approaches that underly recent, significant advances on related problems in materials design. The framework we present here for problems in morphogenesis surmounts known design problems including grayscale ambiguity, manufacturing inaccuracy, and artificially over-specified criteria. Our results give examples where coarse-grained molecular methodologies can be used to derive results for macroscopic design problems

Advances in material model calibration for computational solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A FRAMEWORK FOR CONTEXT-SPECIFIC CONSTITUTIVE MODEL CALIBRATION

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ABSTRACT

Virtually all modeling and simulation relies critically on the calibration of model parameters that describe the behavior of a physical system under different environmental conditions and loads. However, approaches to obtaining and validating optimal parameter values vary widely due to differences in available data, material physics, simulation codes, and user experience. There are many aspects to the problem of developing such an approach, but one that has received relatively little attention is transferability. It is common to think of a set of parameter values as optimal in the global sense that a model best fits given data with a this single set of values. The canonical example is calibration to minimize the sum of squared error between the model output and some set of observations. In this paradigm, the calibrated model itself is transferable from one context to the next. Contrary to the assumption that there exists a single, context-independent optimal model calibration, engineering practice clearly demonstrates that different model calibrations to the same data can be optimal for different end-use scenarios. With this in mind, we propose a calibration scheme that takes into account the end use, and can be repeatedly applied to the same input data to achieve model calibrations that are optimal for specific contexts. In this paradigm, it is the approach that is transferable between contexts, rather than the calibrated parameter values. We demonstrate the efficacy of this framework with simple but relevant problems in elasto-plasticity.

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Current trends in phase-field modeling and computations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPLORING VASCULAR WALL FRACTURE THROUGH AN INTEGRATED EXPERIMENTAL AND NUMERICAL APPROACH

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ABSTRACT

Vascular tissue fractures play a crucial role in cardiovascular events like strokes, and aortic dissection, major causes of global death and disability. A better understanding of vascular tissue fracture, therefore, bears the potential to improve the treatment of vascular patients and optimise medical device designs. In addition to robust in-vitro experiments, the identification of fracture mechanical properties relies on robust and efficient numerical tools.
We present different Finite Element Method (FEM) approaches to model vascular tissue fracture focusing on the symmetry-constraint Compact Tension (symconCT) test, an in-vitro test protocol to study vessel wall fracture [1]. Our numerical models represent the fracture by (i) cohesive zones placed at finite element facets [1], (ii) cohesive zones embedded within the finite element following the Partition of Unity FEM (PUFEM) [2], and (iii) the phase-field approach [3].
Regardless of very good agreement with the recorded experimental data, the approach reported in (i) revealed an excessively large cohesive fracture length of 11.4 mm at which complete separation was observed. Important rate-dependent dissipation mechanisms in the fracture process zone might, therefore, have been overlooked, and the embedded formulation (ii) incorporated additional dissipation in the traction separation law. Towards avoiding challenges related to the dynamic introduction of the cohesive zone elements according to approach (ii), a phase-field model was implemented in FEAP (University of California at Berkely), comprising approach (iii).
The numerical efficiency and robustness of the investigated approaches are explored, and the plausibility of model predictions is discussed in relation to experimental observations of the symconCT test results. As the primary aim of our work was the comparison of different numerical methods, an overly simplified vessel wall description was used. Fundamental mechanisms associated with the inception and development of damage, leading to tissue failure, are not explicitly described. Irreversible tissue description that incorporates the time-dependent failure mechanisms across length scales might provide more realistic insight into vascular tissue failure.

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Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING THE TARGET ANTIGEN HETEROGENEITY IN IMMUNOTHERAPY WITH CAR-T CELLS

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ABSTRACT

Immunotherapy with chimeric antigen receptor T-cells (CAR T cells) is a recent cancer treatment approach, wherein T lymphocytes are extracted from the patient, genetically manipulated to recognize the specific antigen expressed by the patient's tumor cells, and expanded in culture. Upon reinfusion into the patient, these cells are capable of identifying and eliminating cancer cells expressing the targeted antigen. Despite the success of this adoptive therapy against various cancers, mainly those of the hematopoietic system, the durability of remission has been the subject of recent research. Studies have indicated that the immune pressure resulting from CAR T cell immunotherapy induces changes in antigen expression by cancer cells, such as antigen loss or reduction in expression. Eventually, antigen expression may drop below the level necessary for CAR T cells to recognize cancer cells, compromising the durability of the therapy response [1].
Building on a groundbreaking study [2], this study entails developing a series of mathematical models employing integral-partial differential equations to investigate the influence of antigen-mediated resistance mechanisms on therapy outcomes. Tumor cells are assumed to exhibit heterogeneity in terms of antigen expression density, represented as a continuous variable influencing the dynamics of CAR-T cell in vivo expansion and cytotoxicity, encompassing bystander effects. The investigation delves into the contribution of these mechanisms across various biological scenarios, including pre-existing antigen-negative cancer cells and mutations, contributing to a more profound comprehension of pivotal factors influencing resistance to CAR-T cell immunotherapy, as well as assessing the validity and predictability of the developed models in the presence of uncertainties.

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TIME-STEPPING FOR NONLINEAR BIOLOGICAL TISSUES: IS FIRST ORDER ENOUGH?

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ABSTRACT

Biological tissues are complex, heterogeneous materials. In the case of skeletal muscle, the quasi-incompressibility of the tissue brings computational challenges that, while known and understood for quasi-static simulations, are still open problems for fully dynamic simulations.

In this talk, we present some recent results regarding time-stepping schemes for finite-element formulations of hyperelasticity. In particular, we discuss the influence of the order in which the variables are discretized (Rothe's method vs. method of lines), as well as the performance of some traditional second-order schemes.

Inverse and optimization problems for advanced materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADJOINT-BASED INVERSION FOR FRICTIONAL PARAMETERS IN EARTHQUAKE SIMULATIONS

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ABSTRACT

Earthquake cycle and dynamic rupture simulations are promising tools to better understand earthquake nucleation and seismicity. The bulk of the solid Earth is modeled by appropriate partial differential equations of elasticity. Fault friction is modeled by rate-state friction laws, which involve nonlinear relations between fault tractions, slip velocity, and state variables that capture the dependence of frictional strength on the slip history. However, parameters of the friction law, as well as initial stresses, are generally unknown and difficult to constrain. Determining frictional parameters and initial stresses requires inverting seismic and/or geodetic data. The inversion is a PDE-constrained optimization problem where we seek parameter values that minimize the misfit between model output and data.

We propose a gradient-based optimization, where the gradient of the misfit is efficiently computed by solving the adjoint problem. We show that, for linear elasticity coupled to nonlinear rate-state friction, the adjoint problem consists of the same linear elasticity equations, but with linearized rate-state friction. The adjoint friction law and state equation include time-dependent coefficients that are functions of slip velocity and state from the forward problem. Only a special case of this method has been derived previously, for quasi-dynamic cycle models with a boundary element discretization of the linear elastic slip-stress change relation [Kano et al., 2013].

To discretize the elastic wave equation, we use summation-by-parts (SBP) finite differences. The fault interface conditions are imposed weakly, using simultaneous approximation terms (SAT), which are based on characteristic variables to avoid excessive stiffness from the friction law [Erickson et al., 2022]. We prove that this SBP-SAT discretization is dual-consistent, meaning that the adjoint of the discretized forward problem is a stable and consistent discretization of the adjoint problem. Additionally, the computed gradient is the exact gradient of the discrete misfit functional as well as a consistent approximation of the continuous gradient. The former is demonstrated by numerical simulations with a rough fault. Numerical inversions with synthetic data further show that the method is indeed capable of determining frictional parameters.

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Modeling and simulation of advanced manufacturing processes for metals
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DESCRIPTION, VERIFICATION, AND VALIDATION OF A THERMO-FLUID SOLVER FOR LASER POWDER BED FUSION MELT POOL SCALE PREDICTIONS

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ABSTRACT

The Laser Powder Bed Fusion (LPBF) process is an additive manufacturing technique which achieves consolidation of metal powder using a laser to selectively melt, layer-by-layer, parts of a powder bed. At the melt pool (MP) scale, driving forces include laser heating, solid-liquid phase change, evaporation, and surface tension. Evidence shows that reliable numerical predictions of MP evolution require thermo-fluid solvers modeling all the aforementioned terms [1]. These terms induce strong coupling between the governing equations, requiring additional considerations to ensure accurate resolution. However, few LPBF publications report a complete description of their frameworks: assumptions are not stated and the solution sensitivity to the space and time discretization is rarely assessed. This makes it difficult to reproduce the results and assess their adequacy.

This work provides a thorough description of the open-source thermo-fluid Finite Element (FE) solver Lethe, focusing on its application to MP scale simulations. It features verified and validated solvers required to solve the energy and incompressible Navier-Stokes (NS) equations. It also implements a Volume of Fluid (VOF) method for the evolution of the liquid-gas interface and adaptative mesh refinement to ensure sufficient discretization.

Lethe uses a monolithic approach for the NS equations resolution and implements the continuum surface method to model the fluxes at the liquid-gas interface. Required surface normal and curvature are computed from the VOF solution using L2 projections, thus reducing parasitic velocities. Phase change is resolved using the energy equation, considering implicitly the enthalpy change through the specific heat capacity and latent heat of fusion contributions. Viscous and/or Darcy penalization model the stasis in the solid and drag effects in the mushy zone. The laser heating is a Gaussian heat flux and the evaporation cooling is implicitly treated.

The solution’s sensitivity to space and time discretization is presented for static, rising, and thermocapillary droplet cases and capillary wave propagation benchmarks. Finally, results for LPBF cases are presented, focusing on the time evolution of the MP dimensions for the stationary and moving laser irradiation of bare plates presented in the experimental work of Cunningham et al. [2]

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Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN MULTISCALE MODELING

NR Aluru[1]*

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ABSTRACT

The breakdown of classical constitutive theories for problems in mechanics (fluids, solids, thermal, etc.) at the nanoscale require the inclusion of electron correlations and atomic scale interactions. Furthermore, in many areas of mechanics, new physics arises at small scales that makes the use the continuum theories questionable. These, and many other issues, require the development of theories and computational approaches that seamlessly integrate physics from the quantum scale to the continuum scale to accurately resolve the length and time scales encountered in nanomechanics problems. This talk will focus on two aspects – first, we will discuss how deep learning can be used to bridge ab-initio to continuum scales. As a demonstration example, we will show how the structure of confined soft matter can be accurately resolved using deep learning-based multiscale theory. Second, we will demonstrate that deep learning methodologies can be used to model problems involving phenomena such as electron transfer processes, chemical reactions, and transport.

TOWARDS THE INVERSION OF GEOPHYSICAL DATA GENERATED WITH PARAMETRIC PDES THROUGH DEEP LEARNING

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ABSTRACT

Deep learning (DL) techniques have become more powerful for simulating and inverting geophysical problems, enabling fast real-time solutions to invert problems by training Deep Neural Networks (DNNs) (see, for instance, [1,2]).

However, to produce reliable and robust results, DL methods need customized design choices specific to the problem being solved and the available data. Indeed, one of the main challenges is obtaining sufficient data that connects variations in the problem's model parameters with the solution of the forward problem, which is often stated as a Partial Differential Equation (PDE).

Thus, this work analyzes the impact of the quantity and quality of the data on DL inversions and also examines how the selection of the loss function might affect the results. For that, we generate synthetic measurements for problems with geophysical interest using a massive data generator based on a Goal-Oriented hp-adaptive Finite Element Method (FEM) [3]. Our initial findings suggest that this approach can provide valuable insights for solving inverse problems with DNN techniques that require data.

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Machine learning for large scale models in physics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GRAPH NEURAL NETWORK FOR LARGE-SCALE GRAPH PREDICTION OF SHELL BUCKLING

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ABSTRACT

Predicting buckling loads in spherical shells is essential in a wide range of applications, from industrial tanks and pressure vessels to critical aerospace engineering components. Buckling is highly sensitive to defects or geometric variability, as characterized by the knockdown factor (reduction in buckling load for imperfect shells). For non-trivial shells this factor is an empirical value – the ratio between the measured buckling load and the prediction for a perfect shell [1]. However, the testing procedure is usually destructive and unsuitable for practical applications. Circumventing the experimental route became possible with the advent of finite element analyses, as these simulations can reliably predict the knockdown factor when the geometry is known in detail. Nevertheless, obtaining predictions for practical shells with multiple defects still involves significant computational resources [2].
We created Graph Neural Network (GNN) surrogate models to address this challenge by leveraging GNNs' ability to predict the buckling response efficiently. We explore the benefits of GNNs in reducing mesh dependency and handling arbitrary and complex domain shapes. We also characterize GNNs' limitations, particularly in dealing with large node numbers, proposing a practical strategy that properly balances between mesh refinement and the integration of far-field phenomena [3]. We demonstrate the advantages of the proposed strategy in the context of buckling of spherical shells, but we believe that the methodology is applicable in different contexts.

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Computational modeling of extreme-loading events
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VALIDATING 3-AXIS MECHANICAL SHOCK ENVIRONMENTS WITH NONLINEAR DYNAMIC MODELS

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ABSTRACT

It is important to confirm components and systems will survive their intended environments through testing before the system is finalized. Additionally, it is more cost effective to perform component tests throughout the design process. These components are tested in the laboratory and are commonly tested uniaxially. However, it is possible that a uniaxial test requires a larger input force to reach the desired response than a 3-axis response would require. The larger force in the uniaxial test can cause damage to the component, even though the real input from the environment would not case the damage. Multi-axis testing is therefore desirable, though it is more complicated and time consuming for test engineers to design and calibrate the test fixtures to reach the desired loads. To improve the test design process, the test fixture can be modeled computationally to quickly iterate through designs. In extreme shock environments, it is important to capture the nonlinear behavior of the system. These nonlinear features include large displacements, nonlinear material behavior, contacts, preloads, and friction. Shock tests examined in this work are performed by launching an aluminum projectile from an air gun into a resonant plate fixture to impart the shock into the unit under test that is mounted on the plate. In the explicit dynamics analysis procedure initial velocity is applied to the projectile and collision of the projectile and plate is simulated. This process allows to avoid any simplifying assumptions, including approximations of the input force. It has been discovered that results are sensitive to the models used to represent nonlinear materials such as felt and rubber, that are utilized for tuning of the input forces. Special attention has been paid to tuning those models to achieve desired behavior, particularly with respect to damping characteristics. This presentation explores effects of those materials and other nonlinear characteristics as well as various other features of the model. Commonly depreciated aspects of the model, such as threaded inserts or the preload of bolts, are modeled to evaluate their necessity to the model. Simulation results are compared to the test data. Validating the modeling methods used will ensure trust for future test fixture designs.

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Data-driven methods for modeling complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NON-LINEAR DIMENSIONALITY REDUCTION METHODS IN NON-NEWTONIAN FLUID MECHANICS

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ABSTRACT

Simulating complex fluid dynamics involves computational challenges, such as the numerical solution of full-order models associated with parametric nonlinear partial differential equations. In recent decades, the construction of reduced-order models based on machine learning techniques has emerged as an elegant alternative to mitigate the computational costs associated with solving high-dimensional problems. In this context, dimensionality reduction methods are crucial for managing with the reduced coordinates extracted from data.

Nonlinear dimensionality reduction methods offer advantages in comparison with traditional techniques adopted in fluid mechanics, like Proper Orthogonal Decomposition (POD). In general, these nonlinear strategies achieve effective reconstructions with minimal mode usage. Autoencoders (AE) stand out as a common nonlinear dimensional reduction method across various applications. Additionally, Kernel Principal Component Analysis (KPCA) serves as an alternative nonlinear method, extending the capabilities of POD through non-linear kernels. It is worth to notice that both linear and nonlinear methods have been widely applied in the context of Newtonian fluid flows [1].

By considering a class of non-Newtonian fluids, known as viscoelastic fluids, our study demonstrate that nonlinear methods capture dynamics in a way that reconstructions preserve essential characteristics, such as the mechanical energy of the problem. This is particularly significant for viscoelastic flows, where elastic energy is often overlooked in favor of kinetic energy during reconstructions. This aspect also highlights the importance of choosing the right metric when working with different types of flow. Furthermore, viscoelastic problems presents a set of new parameters for the fluid, leveraging the interest for parametric reductions, which the non-linear models also shows better results when compared with POD.

The selection of an appropriate method extends beyond accurate reconstructions; it significantly influences downstream applications, such as reduced order models. We illustrate how the careful selection of nonlinear methods can enhance reconstructions, facilitating the application of reduced order techniques like Sparse Identification of Nonlinear Dynamics (SINDy).

Our study contributes to the discussion of viscoelastic fluid flows by comparing linear and nonlinear dimensionality reduction methods. The use of nonlinear kernels may recover more information due to the nonlinear nature of the problem, shedding light on the nuances between linear and nonlinear approaches.

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Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICS-GUIDED HEAT SOURCE FOR TRANSIENT LASER ABSORPTANCE PREDICTION IN METAL ADDITIVE MANUFACTURING

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ABSTRACT

In the realm of Laser Powder Bed Fusion (LPBF) Additive Manufacturing (AM), properly quantifying laser energy absorption is a pivotal and requisite first step for accurately simulating the physics of laser-material interactions. Because, when higher laser energy is observed in other words, at higher Volumetric Energy Density (VED), a vapor depression zone (keyhole) form. This formation of keyholes significantly influences the energy absorption rate, the melt pool dynamics and, ultimately, the quality and properties of the as-manufactured part. The traditional approach for modeling and predicting laser energy absorption is purely physics-based and employs ray tracing to determine the laser ray paths. Although effective, this approach is computationally expensive and thus presents significant practical challenges when applied to part-scale analyses. Thus, to advance the state of the art in simulating the LPFB AM process, there is a need for novel modeling approaches that better balance high-fidelity capture of laser absorption with practical levels of computational expense. To address this compelling research opportunity, we have developed a “physics-guided laser heat source,” an innovative solution designed to approximate and replace the resource-intensive ray tracing method. This approach involves an in-house-developed C++ code that employs physical laws derived from synchrotron X-ray visualization (solved by the Finite Volume Method (FVM)) coupled with sphere radiometry measurements for a more accurate laser heating model. Predictions obtained from our new physics-guided heat source are compared to (a) a physics-based simulation using ray tracing in ANSYS and (b) experimental measurements under seven different test conditions on a powderless bare IN718 plate. Our results exhibit excellent agreement with both the experimental data and the physics-based model, achieved at an order of magnitude lower computational cost. This advanced yet more efficient computational modeling approach is poised to significantly enhance the simulation of multi-layer and multi-track scan paths in LPBF processes. Consequently, the developed method holds great promise for accurately simulating part-scale LPBF processes, including keyhole porosity and lack-of-fusion porosity.

Improving the efficiency and accuracy of computational methods through machine learning
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPLORING TRANSIENT FLOW IN PORE-SCALE POROUS MEDIA: A DEEP LEARNING PERSPECTIVE ON THE METAL FOAM HEAT EXCHANGER'S ANALYSIS

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ABSTRACT

Predicting flow in pore-scale porous media is pivotal across diverse scientific and industrial fields due to its impact on the intricate dynamics of microscopic fluid movements. For instance, in environmental engineering, the pore-scale flow prediction plays a crucial rule for devising effective pollution control and remediation techniques. The current study aims to develop a hybrid training dataset that incorporates turbulent numerical simulation results and experimental data to predict the transient flow behaviour and thermal performance of a metal foam heat exchanger. This prediction is accomplished through the application of a deep forward neural network-boundary condition (DFNN-BC) model. A novel approach is presented for predicting the passage of transient flow through pore-scale porous media (PSPM), covering a broad range of two input parameters namely, Reynolds number ($4{,}000 < Re_{inlet} < 20{,}000$) and pore per inch ($1 < PPI < 40$). The achievement of this objective necessitates precise metal foam geometry as a crucial prerequisite for the analysis. The extraction of the three-dimensional (3D) geometry of metal foam is carried out by employing a convolutional neural network (CNN) on a series of metal foam images. The Optimized CNN architecture consists of 14 layers with learnable weights, where a rectified linear unit (ReLU) activation function is utilised to introduce nonlinearity. Following the provision of the 3D geometry and the validation of the CNN approach, a high-fidelity and double turbulence model based on finite volume (FV) simulation is applied to a localised region of a heat exchanger that incorporates metal foam. The simulation employs the large eddy simulation (LES) method to capture transient flow through the metal foam, while the Reynolds average Navier-Stokes (RANS) model is employed to characterise the flow over the pore-scale porous media (PSPM) and within the free stream. To address the challenges posed by the intricate PSPM, the prediction method updates the boundary condition during each iteration of the loss function solution. Following the validation of the DFNN-BC emulated results using experimental data, the heat transfer coefficient and pressure drop of the metal foam heat exchanger for the entire domain are estimated.

Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FINITE ELEMENTS AND MATRIX STRUCTURAL ANALYSIS

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ABSTRACT

This reflection centers on a memorable encounter with Professor Reddy in the late Professor Ernest Hinton's office at Swansea University, Wales, UK, in 1994, highlighting the profound impact of Reddy's seminal book on the finite element method. Beyond reminiscence, this article aims to address a pervasive issue in computational mechanics, particularly in material design and nanotechnology fields.

The prevalent terminology of solving truss or frame structures by the 'finite element method' (FEM) has become widespread, creating challenges in dispelling the misconception that structures comprised of prismatic members are and should be addressed using finite elements. The root of this issue lies in finite element textbooks that often fail to differentiate between the 'matrix analysis method (MAM)' and the FEM. Even notable works, such as Professor Reddy's excellent book on FEM, inadvertently conflate these two different techniques.

While both MAM and FEM share similarities in forming member equations in matrix form, assembling them, and solving the resultant system of equations, they differ in the following:
1- MAM is used for discrete structures, while FEM is devised for continuum problems.
2- Contrary to the MAM, in the FEM, the domain of the problem is artificially divided into elements, creating the FE mesh.
3- In analyzing skeletal structures, in MAM, the components of member stiffness matrices are obtained from force-displacement (including moment-rotations) relations. In FEM they are resulted from the assumed shape functions used for the approximation of general displacements, which are polynomials without inherent physical meaning.
4- MAM yields exact solutions, while FEM solutions are approximations. For instance, in an Euler-Bernoulli beam under uniform loading, the exact solution involves a fourth-degree polynomial, whereas FEM approximates it with piecewise cubic functions. This discrepancy is even more pronounced in internal forces and stresses. Another example, exemplified in textbooks, is the suggestion of the need for finite element nodes at locations of point loads on beams. In MAM, by obtaining the end member general displacements and forces the exact solution will be achieved, using statics and strength of materials,

Due to Professor Reddy's significant influence in the community, the author seeks his insight and invites him to write a short note on this issue, which has caused ambiguity in the field.

Imaging-based methods in computational medicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICS-BASED IMAGE REGISTRATION USING NEURAL ORDINARY DIFFERENTIAL EQUATIONS

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ABSTRACT

We present a machine-learning framework for registering medical images, where the satisfaction of equilibrium equations in the large deformation regime is the center of attention. In this regard, a multi-objective optimization problem consisting of: i) a predictor step that maximizes a metric of similarity between the registered and target images, ii) a corrector step that minimizes the total potential energy subjected to Dirichlet boundary conditions given by the predictor step.
The equilibrium equations are fulfilled in a weak sense in the corrector step, where a Dirichleth boundary value problem defines the physics problem, with the Dirichlet conditions coming from a predictor registration step. In this regard, analogous to the finite element method, we minimize the potential energy corresponding to the Dirichlet boundary conditions defined by the predictor deformation field. This type of solution procedure avoids us dealing with the calculation of the second-order derivatives existing in the strong format of the equilibrium equations. Additionally, since the fully connected neural networks are not inherently invertible transformations, we rather use neural ordinary differential equations (NODEs). This architecture has strong expressibility, while the invertibility is guaranteed when a small enough time-step is taken in the NODE discretization.
The structure of the presentation is as follows: firstly, we will overview the fundamentals of the large strain theory of elasticity as well as the basis of the finite element schemes that employ similar predictor-corrector schemes to solve the weak form of the governing equations. Subsequently, we describe the main steps of the new method, i.e., the predictor and corrector steps. Several numerical examples are then discussed to highlight the features of the new technique and to understand the registration and physics problems in depth. We extend the formulation from problems of nonlinear elasticity to account for growth and remodeling, which are essential phenomena in describing medical images of living systems. The framework for growth and remodeling is the kinematic split of the deformation gradient into growth and elastic deformations, with the growth component obeying rate equations based on mechanobiology knowledge, and the elastic component contributing to the elastic energy. Finally, we apply the new method to problems of interest: zebrafish wound healing analysis from confocal images, brain atrophy from MRI data, and skin growth from 3D photographs during tissue expansion procedures.

Multiscale modeling of dynamics in complex media and metamaterials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NON-HERMITIAN DEGENERACIES IN BAND STRUCTURE AND MODAL CHIRALITY OF IN-PLANE STRESS WAVES IN LAYERED MEDIA

Alireza Amirkhizi[*1] and Vahidreza Alizadeh*[1]

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ABSTRACT

We study the coupled in-plane wave propagation in layered media with and without linear loss. Using the transfer matrix method, the band structure as well as the modal behavior of such systems are determined. For lossless cases multiple examples of non-Hermitian degeneracies of the band structure (i.e. of the dynamic operator K/M endowed with Bloch-Floquet periodicity and parameterized by the frequency and wave vector component parallel to the layers) are shown with diverse characteristics. In such cases, two neighboring exceptional points bookend an interval with broken phase symmetry. The interval is generally a stop band but it is shown to appear both in double pass bands as well as double stop bands. The chirality of the broken phase modes will be presented and discussed. Scattering off finite layered systems will also be presented based on the calculation of the scattering matrix from the transfer matrix. Degeneracies of permutated scattering matrix are associated with single-sided non-reflectivity, broken phase symmetry, and potential for lasing, when gain media are utilized. Second order EP pairs are shown to appear when (balanced) gain reaches a threshold. Potential examples for higher order (>2) degeneracies are presented.

Multiscale modeling of dynamics in complex media and metamaterials
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EFFICIENT WAVE MANIPULATION VIA OPTIMIZATION AND MACHINE LEARNING

Feruza Amirkulova[*1], Tristan Shah[1] and Stas Tiomkin[1]*

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ABSTRACT

Efficient wave manipulation via optimization and machine learning
Feruza Amirkulova, Tristan Shah, and Stas Tiomkin
San Jose State University

In this talk, we will present our recent studies on the efficient design of acoustic metamaterials using traditional approaches such as gradient-based optimization methods as well as advanced machine learning techniques such as deep learning and representation learning combined with model predictive control [1, 2]. Specifically, broadband sound focusing, steering, localization, and Willis coupling are the focus of this talk. We will review recent advances and current challenges encountered during the application of gradient-based optimization [3], deep learning, model-free reinforcement learning [4], and generative modeling [5, 6] in an inverse design of acoustic metamaterials. We will summarize and group existing approaches in the inverse design of metamaterials and then discuss current algorithmic limitations and open challenges to preview possible future developments in metamaterial design. We will present numerical examples in both time and frequency domains for arbitrary 2D planar configurations of cylindrical scatterers including fluid, rigid, and elastic scatterers. Proposed frameworks are not limited to 2D planar cylindrical configurations; they can be extended to consider 3D scatterers as well as to study complex acoustic and elastodynamic wave phenomena in non-periodic and periodic media.

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Advances in numerical methods for solution of PDEs
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HIGH-ORDER EXPLICIT PDE SOLVERS USING TRIGONOMETRIC INTERPOLATIONS OF NON-PERIODIC FUNCTIONS (WITH APPLICATIONS TO ENGINEERING, GEOPHYSICS, AND MEDICINE)

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ABSTRACT

This contribution presents recent developments of a Fourier series-based methodology for the numerical analysis of parabolic and hyperbolic partial differential equations (PDEs) with complex boundary conditions. Such a framework is based on a discrete "extension" approach for the high-order trigonometric interpolation of a non-periodic function (i.e., mitigating the notorious Gibb's "ringing" effect), where the ultimate goal is to build high-performance, FFT-speed, dynamic PDE solvers on general (structured, curvilinear) geometries that can provide stable and efficient resolution while faithfully preserving the dispersion/diffusion characteristics of the underlying continuous operators.

In particular, the algorithms presented here extend the class of such methods (known as "Fourier continuation") to encompass variable-coefficient 3D systems, general (curved) 3D domains, 3D parallelization, Neumann-like (e.g., traction or convective flux) boundary conditions, nonlinear/nonstationary (ODE-governed) coupling (e.g., dynamic 0D-coupling), and applications to higher-order PDEs with multiple boundary conditions (e.g., Lagrangian mechanical formulations). The resulting solvers enjoy a number of desirable properties for scientific computation: accuracy by means of relatively coarse discretizations; little-to-no numerical dispersion or diffusion errors; mild (linear) CFL constraints on (explicit) time integration; and efficient parallelization for distributed-memory high-performance computing.

With an eye towards mutual validation of both simulation and experiment, the efficacy of the current state of these tools is demonstrated in the context of some of the collaborative scientific problems that have inspired them, including those in engineering (ultrasonic non-destructive testing and seismic wave propagation [1]), geophysics (seismogenic tsunamis [2]), and medicine (fluid-structure hemodynamics [3, 4], dye diffusion [5, 6]). Performance studies and comparisons to other solvers are additionally presented.

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Multiscale Theory and Modeling of Advanced Nanocomposites
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NEW STRAIGHTFORWARD BENCHMARK SOLUTIONS FOR BENDING AND FREE VIBRATION SOLUTIONS OF CLAMPED NANOCOMPOSITE RECTANGULAR THIN PLATE

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ABSTRACT

This study presents new straightforward benchmark solutions for bending and free vibration of clamped anisotropic nanocomposite rectangular thin plates by a double finite integral transform method. Being different from the previous studies that took pure trigonometric functions as the integral kernels, the exponential functions are adopted, and the unknowns to be determined are constituted after the integral transform, which overcomes the difficulty in solving the governing higher-order partial differential equations with odd derivatives with respect to both the in-plane coordinate variables, thus goes beyond the limit of conventional finite integral transforms that are only applicable to isotropic or orthotropic plates. The present study provides an easy-to-implement approach for similar complex problems, extending the scope of finite integral transforms with applications to plate problems. The validity of the method and accuracy of the new solutions that can serve as benchmarks are well confirmed by satisfactory comparison with the numerical solutions.

Multi-scale and machine learning-based modeling methods for optimization and design of composites
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE ABLATION ANALYSIS FOR REUSABLE AEROSPACE VEHICLE WITH MACHINE LEARNING POTENTIALS

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ABSTRACT

Atomic oxygen bombardment is a major threat of degradation of surface materials on reusable spacecraft that pass through the low earth orbit segment. Therefore, ultra-high temperature ceramics (UHTC) have received increasing attention as a potentially promising material to minimize the degradation caused by atomic oxygen impact of surfaces. However, experiments to measure the performance of surface materials in the LEO environment are very difficult and expensive, so it is necessary to build a computational simulation performance evaluation technology that can replace such experiments. As part of this computational analysis, molecular dynamics simulation is attracting attention because by understanding and analyzing material behavior at the atomic level, it is possible to understand the oxidation behavior of surface materials by simulating the collision of atomic oxygen, which is considered to be a major degradation factor of surface materials, and identifying the oxidation mechanism. For molecular dynamics simulation at the atomic level, it is necessary to use a potential that can simulate chemical reactions between atoms called a reactive force field, which can simulate the degradation process caused by atomic oxygen.

The biggest problem of reactive force fields is that there is no potential that simulates the interaction between UHTCs and oxygen, and developing one requires a large amount of quantum chemistry data and a variety of techniques to optimize it. This has the problem of being very costly in terms of time. In order to increase the accessibility of potential development and secure potentials that can simulate chemical reactions between various elements, this study utilized an open source (SIMPLE-NN) that can generate an interatomic machine learning potential. This code uses the (ASE) package, an atomic simulation environment package, TensorFlow, and supports an in-house code for the quasi-Newtonian method. It also features a weighting system based on a Gaussian density function and can develop potentials that are compatible with a molecular dynamics simulation environment called LAMMPS. In the pursuit of formulating a machine learning potential for the improved simulation of ablation on surface materials as candidates for the exterior of reusable spacecraft, a training dataset was meticulously chosen. An iterative learning strategy was then implemented to ascertain the alignment of machine-learned potential energy surface (PES) values with those energies calculated using Density Functional Theory (DFT).

Verification techniques in computational physics and applied mathematics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

UTILIZING SELF-SIMILARITY FOR SOLUTION VERIFICATION

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ABSTRACT

While most problems in computational physics have no known analytic solutions, there are many problems (or classes or problems) which possess important mathematical symmetries. Self-similarity is a type of mathematical symmetry, which is characterized by the lack of characteristic length or time-scales when an appropriate transformation of variables. For example, the set of hydrodynamic Riemann problems are self-similar (in 1, 2, or 3 dimensions) under a simple transformation $\zeta=x/t$. This self-similarity may be utilized in analyzing numerical solutions, as the discrete solution of the original governing equations (in the laboratory frame) may be transformed to the self-similar frame. Of course, in the discrete system, the temporal and spatial discretization introduces inherent length and time scales (i.e., the grid scale). Thus, while the true continuum self-similar solution ought to be unchanging in time (the self-similarity removes any time dependence), the self-similar transformation of the discrete solution manifests effectively as a time-dependent resolution. That is, the self-similarly-transformed numerical solution appears very poorly resolve at early times, but appears to resolve in time. We apply numerical analysis using this self-similar approach to several common problems, including the triple-point 2D Riemann problem and the Sedov blast wave.

SHAPE-MORPHING NONLINEAR SOLUTIONS FOR MODEL ORDER REDUCTION

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ABSTRACT

We develop methods for fast and scalable computation of reduced-order nonlinear solutions (RONS). RONS is a framework for reduced-order modeling of time-dependent PDEs, where the reduced solution has nonlinear dependence on time-varying parameters. RONS provides a set of explicit ordinary differential equations (ODEs) to evolve the time-varying parameters. These ODEs evolve the parameters so that we minimize the instantaneous error between true dynamics of the PDE and dynamics of the reduced model. Additionally, using the RONS framework, conserved quantities of the governing PDE are easily enforced in the reduced solution. As the number of parameters in the reduced-order solution grows, formation and integration of the RONS equation becomes computationally expensive. To address these computational bottlenecks, we introduce three separate methods: symbolic RONS, collocation RONS, and regularized RONS. These new methods allow applications of RONS to problems which require many parameters in the reduced solution. To demonstrate the efficacy of RONS with these new approaches we consider several numerical examples including simulation of the Kuramoto-Sivashinsky equation and the Fokker-Planck equation in high dimensions. LLNL-ABS-859147

Biomechanics of hard tissues: From experiments and simulations to clinical applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ENHANCING FRACTURE HEALING: INVESTIGATING THE ROLE OF EXTERNAL FACTORS, INCLUDING PARTIAL WEIGHT BEARING AND REHABILITATION, IN ESTABLISHING IDEAL BOUNDARY CONDITIONS

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ABSTRACT

Understanding the intricate interplay of factors influencing the healing process is paramount to optimizing fracture healing. This study addresses interfragmentary movement and focuses on the central role of partial weight bearing, muscle attachments, and rehabilitation exercises in generating perfect boundary conditions for ideal healing. Considering the dynamic nature of the healing phases - from initial connective tissue to fibrous cartilage to soft callus - we define the fracture stimulus thresholds for each phase depending on the fracture situation. As part of this methodology, healthy subjects (n=20) underwent various partial weight and rehabilitation scenarios. In addition, careful measurements were taken to actively record incorrectly adjusted walking aids and over- and under-weight bearing scenarios. To thoroughly investigate the nuanced effects of partial loading and rehabilitation exercises, state-of-the-art instruments include measurable insoles and hand force sensors from novelTM. These instruments actively facilitated the recording of forces during crutch walking, complemented by using EMG sensors by DelsysTM and XsensTM motion capturing system. The individual collected data are integrated into the AnyBodyTM musculoskeletal simulation system, which enables precise joint and muscle forces and moments computation. The collected monitoring data from five patients with tibia fractures now enable the fit customization for each patient. Digital twins of the respective bone-implant systems are generated based on post-operative clinical imaging, with simulations applying the customized boundary conditions. This customization involves identifying the optimal fracture stimulus and interfragmentary movement for every healing phase, every partial weight bearing, and every rehabilitation exercise typical for a tibia fracture. The subsequent integration and evaluation of this diverse data set through musculoskeletal simulations results in a comprehensive understanding of the factors contributing to perfect boundary conditions for fracture healing. Linking local stresses and strains in the fracture gap to the healing window, cf. [1] and [2] and analyzing the healing progress with an inhouse bone healing model based on [3] help to unravel the complexity of the healing process to ultimately develop strategies for optimal rehabilitation and create ideal conditions for fracture healing.

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Multi-scale modeling and upscaling for flow induced vibrations, from local reference simulations to certified industrial tools
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LARGE EDDY SIMULATION OF FLUID/STRUCTURE INTERACTION OF TWO IN-LINE CYLINDERS IN A TURBULENT FLOW

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ABSTRACT

This work reports the numerical results obtained by the CEA with the in-house CFD software TrioCFD within the framework of an OECD/NEA benchmark focusing on the fluid/structure interaction issue. The experimental facility consists of two in-line cantilever cylinders placed in a thin channel and subjected to vibrations under the effect of a turbulent flow. Experimentally, the average and RMS velocity profiles upstream and behind the cylinders, as well as the time signals of pressure, velocity (in fluid) and acceleration (at the top of cylinders) are recorded. The numerical simulations are performed using the wall-resolved large eddy simulation approach. Two grid sizes are considered in order to estimate the mesh sensitivity. The simulations employ a two-way coupling strategy where the fluid and solid equations are solved separately with two distinct solvers, and the fluid/solid interface is tracked with the Arbitrary Lagrangian-Eulerian (ALE) method. More precisely, we employ an explicit Dirichlet/Neumann time marching algorithm working at each iteration as follows:
(i) resolution of the Navier-Stokes equations in ALE formulation with Dirichlet boundary condition at the fluid/solid interface, yielding the fluid forces and the displacement velocity of the mesh points,
(ii) resolution of the structure equations from the Euler-Bernoulli bending beam model with Neumann boundary conditions (imposed loads), yielding the beam velocity,
(iii) the velocity and normal stress continuity is ensured on the fluid/solid interface,
(iv) the beam velocity and fluid forces are exchanged.
The average and RMS velocity profiles computed downstream of the cylinders are found to be in correct agreement with the experimental measurements, even with the coarse mesh. The vortex shedding frequencies for both cylinders are well recovered. Thus provisional results are encouraging. However, at the time of the present abstract, the results of the simulations with the finest mesh are still pending. The average and RMS velocities, as well as the spectra of velocity, pressure, and cylinder acceleration at given points will be further compared to that recorded experimentally.

ACCELERATING ISOGEOMETRIC ANALYSIS WITH JAX: A HIGH-SPEED GPU-POWERED NUMERICAL PDE SOLVER

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ABSTRACT

In this talk, we present a computational framework developed for solving partial differential equations (PDEs) using isogeometric analysis (IGA), leveraging the machine learning framework JAX. Our implementation combines the efficient high order basis of isogeometric analysis with the high-performance computing capabilities of modern GPUs. The solver is designed with a high-level Python interface, inspired by the user-friendly approach of FEniCS, allowing for straightforward formulation and solution of complex PDE problems.

Key features of our solver include its ability to operate at speeds surpassing existing implementations, thanks to GPU acceleration and just-in-time compilation. The solver supports complex multi-patch geometries and various solution strategies, including those based on the weak form (Galerkin method), or the strong form (collocation methods). This versatility ensures that users can select the most appropriate approach for their specific problem, optimizing both accuracy and computational efficiency.

We will demonstrate the solver's capabilities with benchmarks against traditional solvers, showcasing its speed and efficiency. The combination of JAX's automatic differentiation and GPU acceleration with the geometric flexibility of isogeometric analysis opens new avenues for the fast and accurate solution of structural dynamics problems across various scientific domains.

LIMITATIONS OF DISPLACEMENT BASED FINITE ELEMENT METHOD WITH REGARD TO SOLUTION OF PLANE DYNAMICAL PROBLEMS

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ABSTRACT

This work discusses the limitations of displacement based finite element methods with regard to solution of particular types of plane stress dynamic problems. It can be shown analytically that for a finite plate subjected to uniaxial loading, the state of stress at different points in the plate remains uniaxial only if the boundary traction increases linearly with time. It is seen that the lateral strain becomes incompatible when uniaxial state of stress is assumed for the entire plate and the applied boundary traction is harmonic in time. The existing consensus is that the shear and lateral stress components are small in comparison to the applied uniaxial stress, and they can be ignored. To check this assumption, a thin rectangular plate made of a linear elastic material is subjected to uniaxial boundary traction on one end and an appropriate displacement restrain is applied at the opposite end. The traction is temporally varied in linear, sinusoidal and Haversine manner. The appropriate boundary value problem is solved using a commercial displacement based finite element software and a custom multi-field based formulation following the idea in Shankar et al. (2016). The results indicate that the magnitude of the shear stress and lateral stress though small in comparison with the applied uniaxial stress, are nearly 1000 times more than that estimated by the commercial finite element package for sinusoidal and Haversine variation. More importantly, the magnitude of these stresses do not depend on the temporal variation of the boundary traction in case of commercial software but it does in case of the multi-field formulation and analytical solution. This indicates that the results of dynamic analysis using displacement based finite element method should be used with caution.

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Computational mechanobiology of musculoskeletal tissues
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IN SILICO MODELING OF INTRAMEMBRANOUS AND ENDOCHONDRAL OSSIFICATION USING FUZZY LOGIC

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ABSTRACT

The most common type of fracture healing is secondary or indirect bone healing. In this type of healing, both intramembranous and endochondral ossification take place. The latter form of ossification is preceded by chondrogenesis and the mineralization of the formed cartilage matrix. Oxygen and nutrients are transported through the blood and reach specific areas of the fracture callus by the growth of new blood vessels (angiogenesis). The perfusion of blood is a key factor that allows both intramembranous and endochondral ossification to take place. Fuzzy logic (computational) models of fracture healing have been developed since 2000 by Ament and Hofer [1], and a significant contribution has been made by Simon et al. [2], incorporating the perfusion of blood into these models. However, the distinction between soft cartilage and mineralized cartilage, and hence, the mineralization of cartilage and the correct implementation of bone formation through a cartilage intermediate, are lacking. This research incorporates the aforementioned distinction and explores the (negative) interaction between cartilage and angiogenesis. In this model, a set of rules determines the growth of three tissues: soft cartilage, mineralized cartilage and woven bone, along with the perfusion of blood. These rules describe the following processes of fracture healing: angiogenesis, intramembranous ossification, chondrogenesis, cartilage mineralization, endochondral ossification and atrophy. Additionally, the hypoxic nature of cartilage is incorporated by a rule describing vascular resistance. To capture the mechanical loading of the tissues, a finite element analysis is performed and distortional and dilatational strains are extracted. The growth over time is captured by the iterative calculation of all input variables (cperfusion, cperfusion, adj., csoft cart., cmin. cart., cwov. bone, cwov. bone, adj., εdist. and εdila.) and output variables (Δperfusion, Δsoft cart., Δmin. cart. and Δwov. bone). Tissue composition and blood perfusion of surrounding elements are regarded as well for angiogenesis and ossification. An ovine experiment, performed by Claes and Heigele [3], was replicated in terms of geometry, applied axial load and external fixator.
Differences between more rigid/flexible fixation are a result of temporal and spatial differences in the formation of tissues, which are caused by the presence of higher strains in the fracture callus in the more flexible case.

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Multiphase flow and non-Newtonian fluid - Modelling and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL SIMULATION OF THE FOUR-EQUATION TWO-FLUID MODEL FOR ONE-DIMENSIONAL MULTIPHASE FLOW, USING THE FLUX-RECONSTRUCTION (FR) METHOD

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ABSTRACT

In the oil industry, the so-called flow assurance depends on the knowledge of parameters such as speed, pressure and volumetric fractions of the fluids that flow within the production pipelines. Due to the high computational costs involved in simulating flow in oil pipelines, that can have more to 3.0 km length, one-dimensional models are used more frequently in real world applications. Commercial multiphase fluid flow simulators such as ALFAsim and LedaFlow typically uses first-order schemes for the discretization of the advective terms of the flow equations. It is well known that first-order schemes are robust but very inaccurate to the large amount of artificial numerical diffusion introduced. In this context, we propose the use of the very high-order (VHO) flux-reconstruction (FR) method to improve the accuracy and efficiency of the two-fluid model. In our context, the flux-reconstruction method was used to solve the mass conservation equation of the isentropic four-equation single-pressure two-fluid model. To validate the accuracy of our formulation, we present and discuss the numerical results for some benchmark problems. For these problems, our results are very promising and compare quite well with the results found in literature using other classical low and high order methods.

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Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DIRECT NUMERICAL SIMULATIONS OF TURBULENT PULSATING FLOWS THROUGH CURVED PIPES

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ABSTRACT

This study is driven by an investigation into aortic dissection, a cardiovascular disease. Direct numerical simulations using an immersed boundary method[1] are conducted to analyze the hemodynamics within a model of the aorta. Pulsating flows with various frequencies are examined for the aorta, conceptualized as a curved pipe with different radii of curvature. A pulsating flow, with different frequencies, is added to a steady base flow, serving as the inlet boundary condition. The average Reynolds number, based on the time-varying inlet flow, is set at 8000, while Womersley numbers of 22 and 32 are considered. Centrifugal effects cause the peak velocity to shift towards the outer part of the curved section. This phenomenon persists even after the flow exits the curved section, with the peak velocity continuing to be directed towards the outer part. Distinct variations in velocity flow fields and Reynolds stresses are noted for different radii of curvature, whereas doubling the frequency of pulsation yields a less pronounced effect. Dean vortices manifest throughout most of the curved section, with the breakdown of these vortices and the transition to fully turbulent flow occurring at different locations for pipes with varying radii of curvature.

Despite a consistent breakdown mechanism, larger curvature ratio pipes experience an earlier transition to turbulence. The average kinetic energy in a cross-section due to the pulsating component increases along the curved section, indicating heightened kinetic energy at the exit. The outer downstream part of the curved section, representing the descending aorta, exhibits a notably high time-averaged wall shear stress index. Additionally, time-averaged pressure attains a higher value at the outer part of the curved section, implying a positive pressure gradient in the radial direction. The implications of fluid dynamic quantities in the development and progression of aortic dissection are discussed.

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Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A GENERALISED DEEP LEARNING MODEL FOR HOMOGENISATION OF MULTIPHYSICS PROPERTIES OF COMPOSITE MATERIALS

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ABSTRACT

Multifunctional composite materials have gained significant attention in weight-sensitive applications such as the aerospace industry. The optimal design of such materials necessitates evaluation of their multi-physical properties in different loading environments. There exist experimental, analytical and numerical methods for homogenisation of multiphysical composite properties. The experimental approach is highly time-consuming and cost-intensive. Analytical methods can be used for simple cases, but these methods fail to capture the distribution and geometry details of the reinforcements. FEA-based homogenization can be employed to overcome these limitations. Though this approach gives accurate solutions, modelling of statistically equivalent representative volume element (RVE) and choosing appropriate multiphysics boundary conditions is a difficult task. An efficient composite design process requires a simple and faster method for evaluating composite properties. Hence, active research is focused on utilizing machine learning methods to build surrogate models that can predict the properties of interest with the same levels of accuracy as FEA-based homogenization.

Generally, surrogate models are designed to take micro-structure information (in the form of an RVE image, for example) as input and predict its properties [1]. The applicability of the final model depends on the details of the input data or training data, so one must strive to add as much micro-structure information as possible. Further, the existing models developed so far aimed to predict the properties of a single physics as well as a single material system. Having a unified model for predicting multi-physical properties for a wide range of material systems would be beneficial to understanding the response of the composite under various kinds of loads, thus speeding up the design of composites for multi-functional applications. In addition, quite often, surrogate models do not explicitly account for underlying mechanics. The present research aims to embed physics into the surrogate model, an example is the enforcement of homogenisation bounds as a constraint during the model training [2]. In the end, a single physics-respecting CNN-based surrogate model to predict different multi-physical (thermo-elastic, thermal conduction and piezo-electric) properties is presented.

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Analytical models for nonlinear dynamics and evolved dynamics in natural, social and engineering sciences
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXAMPLES OF ANALYSIS METHODS FOR ULTRASONIC VIBRATION-ASSISTED MACHINING

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ABSTRACT

Ultrasonic vibration has been applied to many machining methods and reported to improve machining performance. As examples of machining with ultrasonic vibration, this paper deals with the reduction of welding residual stress, the improvement of machined surfaces in the drilling of laminated materials, and the improvement of machining efficiency in knurling. For each example, the advantages of applying ultrasonic vibration are demonstrated through experiments, and simple analysis methods are proposed to demonstrate the usefulness of ultrasonic vibration.

First, the reduction of residual stress is examined. An experiment was conducted in which welding was performed while ultrasonic vibration was applied. As a result, it was found that tensile residual stress was reduced. Next, since the yield stress near the bead immediately after welding is low, the residual stress was determined by simulation method using a model that takes plastic deformation into account. The results showed that tensile residual stress was reduced for welding while applying ultrasonic vibration. It was also predicted that the higher the amplitude of ultrasonic vibration, the higher the residual stress generated, and the lower the yield stress, the lower the residual stress.

Second, improvement of the machined surface in drilling holes in laminated materials was investigated. Experiments were conducted to drill holes in laminated materials while applying ultrasonic vibration at different drill rotation speeds and feed rates. As a result, it was found that the surface roughness of the machined surface was improved. Next, since the drill is expected to intermittently drill holes in the laminate material in this process, the impulse due to cutting resistance was calculated using a model that takes intermittent cutting into account. As a result, it was found that the surface roughness was improved when the force product without ultrasonic vibration was smaller than or equal to the force product with ultrasonic vibration.

Third, the improvement of machining efficiency in knurling was examined. An experiment was conducted in which knurling was performed while ultrasonic vibration was applied. As a result, it became clear that the indentation machined became deeper when ultrasonic vibration was used. Next, analysis using a mechanical model that takes into account the plastic deformation of the specimen revealed that the use of ultrasonic vibration deepens the indentation.

DEVELOPING DATA-DRIVEN DISLOCATION MOBILITY LAWS FOR BCC METALS

Nicole Aragon[1], David Montes de Oca Zapiain[1], Eric Rothchild[1] and Hojun Lim[1]*

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ABSTRACT

Body-centered cubic metals, such as tantalum, exhibit complex deformation behavior with a significant strength-dependence on temperature and applied stress. To accurately model these materials, it is critical to incorporate accurate dislocation mobility, a fundamental property that determines several characteristics of the plastic deformation. Experimental measurement of dislocation mobility is exceptionally challenging, thus dislocation mobility is often described by a simple empirical model parameterized by atomistic simulations, such as molecular dynamics (MD). These models typically assume fixed model form and parameters are determined by limited dataset. In this work, we utilize genetic programming to perform symbolic regression to establish a phenomenological dislocation mobility law that can easily be incorporated into mesoscale dislocation dynamics models. The proposed model is trained on a comprehensive dataset of MD simulations that characterizes dislocation velocities as a function of stress and temperature. Finally, to leverage the analytical nature of the developed model, dislocation dynamics simulations using the proposed mobility law will be presented.

Current trends and advances in enriched finite element methods and coupled simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A DISCONTINUITY-ENRICHED FINITE ELEMENT METHOD FOR MODELING FRACTURE GROWTH IN BRITTLE MATERIALS

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ABSTRACT

Enriched finite element methods such as the eXtended/Generalized Finite Element Method (XFEM/GFEM) have become popular for modeling problems with material discontinuities (e.g., composites and fracture). The main advantage as compared to the standard finite element method (FEM) remains the versatility in the choice of discretizations, since in XFEM/GFEM discontinuities are completely decoupled from the finite element mesh. However, XFEM/GFEM is no without issues, which include the need for stable formulations to bound the condition number of stiffness matrices and the shifting of enrichments to deal with nonzero essential boundary conditions. Modeling complex kinematics such as branching and merging of discrete cracks remains challenging and requires an intricate computer implementations. At worst, it is currently not possible in XFEM/GFEM to recover smooth reactive tractions from boundaries with prescribed nonzero displacements.

Here we introduce the Discontinuity-Enriched Finite Element Method (DE-FEM) [1,2,3] as an alternative procedure to XFEM/GFEM for modeling crack growth in brittle materials. While DE-FEM retains the mesh-geometry decoupling virtue of XFEM/GFEM, it addresses all of its drawbacks by placing enriched nodes directly along discontinuities. Most notably, this is done with a straightforward computer implementation that enables complex kinematics, namely the modeling of multiple crack growth with branching and merging. Numerical examples show the capability of DE-FEM in obtaining accurate stress intensity factors—with an interaction integral that considers the interplay among cracks and in capturing crack patterns similar to those observed in the literature.

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DISCOVERY OF EQUATIONS IN HETEROGENEOUS MATERIAL MECHANICS THROUGH MACHINE LEARNING APPROACHES

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ABSTRACT

In this presentation, we explore the complex mechanics of heterogeneous materials, such as fiber-reinforced composites, focusing specifically on the stress fields within these materials. Utilizing the AI-Feynman [1][2] algorithm, our aim is to uncover the intricate relationships between variables and to discover equations that sufficiently represent these dynamics.
Conventionally, stress evaluation of heterogeneous materials has been performed by numerical simulation on a per-case basis. This approach is expensive and resource intensive, especially for probabilistic evaluations.

AI-Feynman creates a dataset that follows the basic equations found in Feynman physics textbooks and identifies the physical equations from the data. In our research, applying the AI-Feynman algorithm to datasets generated from numerical simulations enables us to probe inherent non-linear interactions and dependencies, offering insights into the mechanics of complex heterogeneous materials.

In this presentation, we will introduce the details of the problem setting and the AI-Feynman algorithm. Additionally, we will discuss the results of the equations that have been discovered. In conclusion, the validity and effectiveness of this approach in the mechanics of heterogeneous materials will be discussed.

The significance of this study lies in broadening the application scope of machine learning in engineering. Utilizing AI-Feynman reveals critical variables and their interdependencies under complex stress conditions in materials like fiber-reinforced composites, providing new understandings and unprecedented insights, and potentially contributing to new theoretical comprehensions.

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Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A GENERAL HIGHER-ORDER SHELL THEORY USING ORTHONORMAL MOVING FRAME FOR TRANSVERSELY ISOTROPIC HYPERELASTIC MATERIALS

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ABSTRACT

This study presents a general higher-order shell theory to analyze the large deformation of tubular shell structures made of transversely isotropic hyperelastic materials. The salient feature of this shell is threefold: (i) this shell theory formulation has been done using an orthonormal moving frame (OMF) instead of the classical natural covariant frame, which makes the mathematical formulation relatively simpler even for very complex hyperelastic constitutive relation owing to the orthonormal nature of basis vectors; (ii) General-higher order nature of approximation through-thickness of the shell make it equipped to model the deformation of a thin shell as well as thick shell, and at the same time it also removes thickness stretch associated numerical locking, and (iii) the constitutive relations of transversely isotropic hyperelastic material, both stretch and invariant based, are considered eying application in the vascular mechanics. The displacement field of the line normal to the shell reference surface is approximated by general power series polynomials for single-layer shell structure. Subsequently, the kinematics of the shell for orthonormal basis has been derived. It has been shown by Arbind, Reddy, and Srinivasa in [1] that such a coordinate system makes it possible to represent kinematic quantities, e.g., determinant of the deformation gradient, far more efficiently than the in the classical tensorial representation with covariant basis. This study can be regarded as an extension of [1] for incompressible/compressible anisotropic softshells. Here, for a general shell surface geometry, the weak form finite element formulation of the shell theory is presented. Further, the theory has been applied to large deformation analysis of tubular structures, such as biological tubes, under internal pressure. For incompressible material, incompressibility constraint has been applied via the penalty method and the Lagrange multiplier method. For the post-buckling analysis, a nonlinear finite element formulation considering the arc-length method has also been presented. Various numerical examples are shown to verify and validate the formulation presented in this study.

Keywords: Higher-order shell theory, thin or thick shell structure, transversely isotropic hyperelastic materials, analysis of curved tubular shell.

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Advanced numerical techniques for fluid flow in porous media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A HIGHER ORDER FINITE VOLUME MULTILEVEL WENO SCHEME FOR MULTIPHASE FLOW IN POROUS MEDIA

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ABSTRACT

We present a multi-level weighted essentially non oscillatory (ML-WENO) reconstruction on general computational meshes for solving partial differential equations exhibiting advection and degenerate diffusion. The reconstruction combines stencil polynomial approximations of various degrees, including constants, defined on any set of stencils that need not be arranged hierarchically. The nonlinear weighting biases the reconstruction away from both inaccurate oscillatory polynomials of high degree (i.e., those crossing a shock or steep front) and smooth polynomials of low degree, thereby selecting the smooth polynomial(s) of maximal degree of approximation. We also give a general result for determining when a stencil polynomial approximation is accurate. The reconstruction leads to a very general finite volume scheme that can handle shocks or steep fronts in the solution. We apply our new ML-WENO scheme to problems in two-phase flow in porous media.

Scientific machine learning for geophysical applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STORMER – A STATE-OF-THE-ART TRANSFORMER FOR MEDIUM-RANGE WEATHER FORECASTING

Troy Arcomano[*1], Tung Nguyen[2], Alex Wikner[3], Matthew Poska[4], Romit Maulik[4], Rao Kotamarthi[1] and Aditya Grover[2]*

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ABSTRACT

Recently, several deep learning-based models for weather forecasting have been demonstrated with skill approaching or even exceeding traditional numerical weather prediction (NWP). These models include Graphcast, Fourcastnet, FuXi, Pangu-weather, ClimaX, and the AIFS, each with vastly different training methods, machine learning architectures, and variables predicted. It is unknown whether these complex architectures are needed or what part of their training protocols are necessary to achieve their impressive results for medium-range weather forecasting.

Here we introduce Stormer, a simple transformer-based model that achieves state-of-the-art performance on weather forecasting with minimal changes to the standard transformer backbone. Using several ablations studies, we identify the key components of previous work as well as develop new methodology, including weather-specific embedding, randomized dynamics forecast, and pressure-weighted loss, to improve deep learning-based weather forecast models. At the core of Stormer is a randomized forecasting objective that trains the model to forecast the weather dynamics over varying time intervals. During inference, this allows us to produce multiple forecasts for a target lead time and combine them to obtain better forecast accuracy. Stormer performs competitively at short to medium-range forecasts and outperforms current methods beyond 7 days, while requiring orders-of-magnitude less training data and compute. We also investigate downstream applications for our newly developed model. Specifically, to perform data assimilation using real, in-situ observations of the atmosphere and for uncertainty quantification using a combined initial condition and model-based ensemble system.

Modeling, optimization and computational analysis of metamaterials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GRADED ARRAYS OF RESONATORS AND MACHINE LEARNING FOR THE RECONSTRUCTION OF ELASTIC WAVE SIGNALS

Luca Iorio[1], Luca Rosafalco[1], Jacopo Maria De Ponti[1] and Raffaele Ardito[*1]*

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ABSTRACT

In the recent literature, it has been proven that graded arrays of resonators can significantly increase the displacement amplitude of the resonating components [1], with important applications in the field of energy harvesting via piezoelectric patches [2]. As a matter of fact, such metamaterials are highly efficient in the localization of elastic waves and in the amplification of local fields. Such a feature is harnessed in the transduction of elastic energy into electrical energy. On the other hand, the array of resonators, equipped with piezoelectric material, could be used as a sensor for elastic waves. The proposed device exploits the aforementioned amplification and the specific circuits connected to the piezoelectric patch, in order to reconstruct the temporal pattern of an elastic wave. To that purpose, we propose an elastic waveguide, in the form of a slender beam, equipped with an array of paired resonators, operating in close proximity to their first resonance frequency. In view of the rainbow effect, the elastic signal is physically separated into its frequency contents, with a selective excitation of the elements in the array. The piezoelectric patches on each pair of resonators are electrically connected in series, so that it is possible to halve the number of output channels and to double the generated current. The analysis of the signal retrieved from each pair of resonators is carried out by means of an encoder-decoder model, that is designed with the aim of reconstructing the input signal. The typical computational schemes of machine learning are adopted. The selective amplification enables the development of a wave analyzer with an increment of the signal-to-noise ratio. The proposed approach can be adopted to reduce the power consumption of the electronic device that are customarily adopted for signal interpretation. The research activity has been carried out with the support of the H2020 FET-proactive Metamaterial Enabled Vibration Energy Harvesting (MetaVEH) project under Grant Agreement No. 952039

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Complex fluid flows in engineering: Modeling, simulation, and optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTI-FIDELITY AND SURROGATE MODELING APPROACHES FOR UNCERTAINTY QUANTIFICATION IN ICE SHEET SIMULATIONS

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ABSTRACT

This work uses multi-fidelity and surrogate modeling to achieve computationally tractable uncertainty quantification (UQ) for large-scale ice sheet simulations. UQ is of utmost importance to enable judicious policy decisions combating climate change. However, high-fidelity models are typically too expensive computationally to permit Monte Carlo sampling. To reduce the computational cost while achieving the same target accuracy, we use multi-fidelity estimators such as Multi-Fidelity Monte Carlo to shift the computational burden onto less expensive surrogate models derived from coarser discretizations and approximated physics. Albeit sufficient to achieve some improvement over Monte Carlo, with the large size and complex geometry of ice sheets like Greenland and Antarctica these surrogates are still expensive to evaluate. To fully exhaust the capabilities of multi-fidelity estimators in face of the intrinsic low-dimensionality of the high-fidelity solution manifold, we would employ projection-based reduced-order models (ROMs). These typically 1) achieve significant computational savings in the order of several magnitudes, 2) guarantee approximation accuracy through established error theory, and 3) remain interpretable through the governing physical equations of the high-fidelity model. However, constructing ROMs via projection requires access to the full-order operators — a significant shortcoming for large-scale ice sheet solvers with legacy codes. We circumvent this requirement with Operator Inference, and lean the intrusive ROM from available full-order data and the structure of the governing equations. Since Operator Inference is sensitive to regularization for high-order polynomial terms, as are present in the shallow ice equations, we employ a nested Operator Inference variant to further exploit the projective structure and lessen the data requirements. We present examples for multi-fidelity simulations of the ice mass loss in Greenland.

Isogeometric methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MIXED ISOGEOMETRIC METHODS FOR HODGE–LAPLACE PROBLEMS INDUCED BY SECOND-ORDER HILBERT COMPLEXES

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ABSTRACT

Through the seminal works of Buffa et al., the fruitful integration of the two discretization paradigms of Isogeometric Analysis (IGA) and Finite Element Exterior Calculus (FEEC) was demonstrated already in 2011. The latter concept explores and provides design steps for the approximation of so-called abstract Hodge–Laplace problems, which, in turn, represent PDEs derived from Hilbert complexes. The introduction of isogeometric discrete differential forms in [1] laid the foundation for discretizing classical de Rham complexes in a structure-preserving manner using B-splines, meaning the discretization of Hodge–Laplace problems derived from de Rham sequences. Although the FEEC theory was developed for general closed Hilbert complexes, and while Hilbert sequences play a role in various physical applications, connecting IGA and FEEC often proves challenging or is sometimes not directly clear. This is especially true for Hilbert complexes that also encompass differential operators of higher orders.

We present two approaches to obtain well-posed discretizations of a whole class of Hodge–Laplace problems using IGA, while maintaining the inf-sup stability condition. We focus on mixed weak formulations of saddle-point structure and second-order Hilbert complexes. In particular, we go beyond the standard de Rham case and demonstrate that ideas from FEEC and IGA are useful for non-de Rham chains as well. A central tool for describing the underlying settings and for choosing the finite element spaces is the Bernstein–Gelfand–Gelfand (BGG) construction considered by Arnold and Hu in [2]. Our approach allows us to incorporate geometries with curved boundaries, which is not directly possible with classical FEEC approaches, and also provides suitable discretizations in arbitrary dimensions. We show error estimates for both approximation methods and explain their applicability in the field of linear elasticity theory. The theoretical discussions and estimates are further illustrated with various numerical examples performed utilizing the GeoPDEs package [3].

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Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFICIENT SENSITIVITY ANALYSIS ON A SIMPLE LASER POWDER BED FUSION BUILT USING HYPAD-FEM

Juan-Sebastian Rincon-Tabares[1], Mauricio Aristizabal[1], Arturo Montoya[1], Harry Millwater[1] and David Restrepo[1]*

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ABSTRACT

Metal Laser Powder Bed Fusion Additive Manufacturing (LPBF-AM) is revolutionizing the global manufacturing industry due to the design flexibility of the process that allows fast innovation and production of optimized complex-shaped components. However, the transformative potential of LPBF-AM remains unrealized due to the need for reproducibility and reliability. These pitfalls create uncertainty in the performance of the fabricated parts due to the unmeasured influence of LPBF-AM process parameters. Modeling and sensitivity analysis have become promising approaches to measuring parameters' influence and overcoming these issues. This study introduces a methodology to perform an efficient sensitivity analysis on a simple build of LPBF-AM. The methodology implements HYPercomplex-based Automatic Differentiation (HYPAD) within traditional FEM formulations (which is known as HYPAD-FEM) to deliver fast and accurate sensitivity solutions [1]. HYPAD-FEM can simultaneously obtain multiple first and high-order sensitivities to initial conditions, load conditions, thermal properties, powder bed properties, or shape with a single average sample [2,3]. Using this methodology, one can exploit the full fidelity of a model to obtain fast and accurate sensitivities from the whole simulation, which are usually limited by computational cost and subtraction errors. The methodology is verified using a model that consists of a laser sequentially melting Ti64 powder layers on top of a bedplate in a rectilinear track. The model can handle property variations due to temperature, phase change, solidification, and a mobile energy beam source. This research is essential for understanding the performance variations due to the process parameters governing the LPBF-AM and determining best practices for improvement. Also, this study provides a crucial step towards enhancing the reproducibility and reliability of LPBF-AM, offering valuable insights for process optimization and part qualification.

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Multiphysics and data-driven modeling for cardiovascular biomedicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTATIONAL MODELING OF HEMODYNAMIC COLLAPSE: INVESTIGATING VOLUME STATUS VARIATIONS IN BLOOD VESSELS USING CFD AND FEA

Nicolas Aristokleous[1,2], Dara Collopy[2], Friedrich Wetterling[2], Fiachra Sweeney[2], Malachy O'Rourke[1] and Eoin O'Cearbhaill[1]*

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ABSTRACT

Accurate assessment of a patient's volume status is crucial in clinical practice, given the significant impact of hypovolemia and hypervolemia on morbidity and mortality rates, especially in heart failure and critical illness [1]. The inferior vena cava (IVC), crucial for systemic venous return, serves as a potential indicator for fluid responsiveness and volume status evaluation, often assessed indirectly through external ultrasound methods. However, the complexity of ultrasonographic volumetric assessment of the IVC, influenced by challenges such as the respiratory cycle, limits its clinical adoption. Understanding the intricate interplay between the respiratory cycle, IVC geometry, and collapse is essential for accurate interpretation.

This study aims to investigate collapsible tube phenomena, focusing on an idealized geometry resembling the IVC. We develop a numerical simulation framework to accurately represent IVC physiology and examine alterations in collapse across three distinct volume statuses: euvolemia, hypervolemia, and hypovolemia.

The idealized IVC model construction and computational solid and fluid models were conducted using ANSYS Workbench 2021R2, employing Mechanical and Fluent as solvers for structural and fluid dynamics, respectively. The IVC wall behavior was simulated using an isotropic, incompressible, 3rd order Ogden hyperelastic material, with external abdominal pressures during expiration and inspiration modeled with a constant pressure distribution applied to the outer wall.

We present a qualitative comparison of model deformation across different volume statuses and respiratory phases, revealing significant deformation in hypovolemia during both inspiration and expiration, while hypervolemia results in vessel expansion due to negative transmural pressure. Notably, euvolemia demonstrates distinct differences in inspiratory and expiratory areas compared to hypovolemia and hypervolemia.

The computed Pressure-Area curves provide valuable insights, with euvolemia displaying significant changes between respiratory phases. The agreement between our results and literature findings validates the reliability of our simulations [2,3].

In conclusion, this study offers foundational insights into the biomechanics of IVC-like vessel collapse, paving the way for further research to refine computational models, enhance clinical applicability, and deepen our understanding of collapsibility dynamics in various physiological and pathological contexts. Additionally, we are currently working on performing the same study with more realistic simulations by

implementing patient-specific data, which will not only enrich our findings but also help validate the robustness of our results.

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Scientific machine learning for geophysical applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATION OF VARIATIONAL DATA ASSIMILATION TO HIGH-SPEED OUTFLOW BOUNDARY-VALUE PROBLEMS OF THE IDEAL MAGNETOHYDRODYNAMICS EQUATIONS

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ABSTRACT

Over the last several decades, considerable effort has been devoted to the development of accurate and efficient simulation methods for a range of space-physics phenomena based on global magnetohydrodynamics (MHD) descriptions and the solution of the equations of ideal MHD. Some notable examples include [1, 2, 3]. Despite the sophistication of these techniques, their accuracy in practice is very often limited by uncertainties in model input parameters. These uncertainties can become particularly evident in the forecasting of transient space-weather events, where the specification of appropriate initial and boundary data can be a significant challenge. The application of data assimilation techniques in which observational measurements are incorporated to constrain model uncertainties offers a means of improving the predictions of global MHD models. To this end, this study presents the first application of a variational-based data assimilation strategy to boundary value problems for the three-dimensional ideal MHD equations, with a systematic treatment for the solenoidal constraint associated with the magnetic field. In the proposed approach, synthetic in-situ data for prototypical steady high-speed MHD outflows representative of the solar wind are considered and model-data mismatch is efficiently minimized via an optimization procedure that makes use of a discrete adjoint method in the evaluation of model parameter gradients. Details of the finite-volume solution method for the ideal MHD equations as well as the data assimilation algorithm for the inner boundary data of the MHD outflows will be provided. Additionally, a number of observing system simulation experiments will be presented, demonstrating the error-reduction capabilities of the proposed variational data assimilation framework.

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Architected materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MECHANICS INFORMED RECONFIGURATION AND MEMORY FORMATION IN SOFT MULTISTABLE STRUCTURES

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ABSTRACT

Shape adaptation in materials and structures enables multifunctionality by leveraging different geometrical configurations. These multifunctionality and adaptability stem from the property, form, and function relationship in which any variation in one results in changes in the other. One avenue for exploiting this relationship leverages geometrical multistability, the property of a system to exhibit several stable states that depend solely on the architecture independently from the material constitution. One roadblock impeding the implementation of multistable structures into engineering systems is the difficulty of designing functional shapes associated with each of their stable states. A class of multistable behavior characterized by strong order-dependence to inputs (also referred to as non-abelian response), referred to as hierarchical multistable, offers opportunities for embodying reconfiguration and memory. Furthermore, the mechanics of such hierarchical multistable structures inform the possible shapes and memory capacity of such structures, thereby providing a route towards their rational design.
We leverage the underlying mechanics of hierarchically multistable structures to realize physical systems that combine shape reconfiguration with memory formation. We demonstrate the utility of embodying reconfiguration and memory formation for the rational design of soft robots that display the features of temporal finite state machines (FSM) that yield different output shapes depending on the recorded sequence. We show how embodying into the structural response this type of temporal FSM strategy offers a new route for controlling soft robots without sensors and closed-loop control. Exploiting the nonlinear mechanics of multistable structures to the designer's advantage allows for physically embodying memory and computation, thereby providing a blueprint for encoding sense-compute-actuate loops in purely mechanical systems that resemble functions characteristic of the peripheral neural system in organisms.

Machine learning algorithms for accelerating material characterization, discovery, design, and manufacturing processes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BIRDSHOT: A FRAMEWORK FOR THE ACCELERATED DISCOVERY AND OPTIMIZATION OF ALLOYS

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ABSTRACT

In this talk, we present the Batch-wise Improvement in Reduced Design Space using a Holistic Optimization Technique (BIRDSHOT) framework and its application to the efficient discovery of Refractory High Entropy Alloys (RHEAs). BIRDSHOT incorporates the strengths of ICME and combinatorial methods, while addressing all their drawbacks, as it: (i) employs novel machine learning (ML) and data-driven search algorithms to identify efficiently the feasible regions amenable to optimization; (ii) exploits correlations to fuse simulations and experiments to obtain efficient ML models for predicting PSPP relations; (iii) uses Bayesian Optimization (BO) to make globally optimal iterative decisions regarding which region in the RHEA space to explore/exploit, leveraging existing models and data; (iv) is capable of carrying out multiple optimal parallel queries to the design space. In this work, we apply our BIRDSHOT framework to efficiently explore and exploit the RHEA space, with a focus on the accelerated discovery of refractory alloys as potential replacements of state-of-the-art Ni-based superalloys used in gas turbine engines (GTEs). Our work considers a large number of application-relevant objectives and constraints. The framework first reduces the design space through a combination of CALPHAD-based phase stability predictions, physics-based as well as machine-learning models to identify the feasible space amenable for further investigation. Using advanced design-of-experiment protocols, we select an initial alloy set to explore. These alloys are in turn synthesized, homogenized, and processed in order to characterize their mechanical properties (including limited experiments at elevated temperatures) as well as their oxidation resistance. “Digital twins” of the same alloys are investigated using DFT-based calculations. Theoretical criteria for ductility extracted from these calculations are used for further screening of the alloy space. Our framework is further enhanced by augmenting the thermodynamic database using a theory-only high-throughput CALPHAD approach in addition to traditional CALPHAD-based thermodynamic assessment of phase stability based on literature and data generated from our own experimental investigation. Initial data is then fed into an advanced multi-information source, multi-objective, multi-constraint batch-based Bayesian Optimization approach to carry out an iterative search for increasingly improved refractory alloys.

VIRTUAL ELEMENTS FOR THE NAVIER-STOKES PROBLEM ON CURVILINEAR DOMAINS

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ABSTRACT

Advance and application of meshfree methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

URBAN FLOOD MAPPING USING SPH METHOD AND PRECIPITATION DATA BASED ON LIDAR DATA

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ABSTRACT

Urban floods are among the most dangerous and devastating natural hazards with extreme and undeniable consequences. With the recent creation of freely accessible, high-accuracy Light Detection and Ranging (LiDAR) data at 1-meter resolution, one approach to mitigate flood risk involves pinpointing inundated areas through detailed flood mapping. Incorporating the precipitation data can improve the realism and accuracy of flood simulation due to its ability to provide invaluable insights regarding the quantity and spatial distribution of rainfall. Urban flooding's intricate flow patterns, influenced by structures and obstacles, challenge traditional Eulerian models. Smoothed Particle Hydrodynamics (SPH), a meshfree approach, offers a possible solution as it mitigates grid generation and mesh distortion issues.

This study aims to identify inundated areas by producing flood mapping using the SPH method and LiDAR data. DualSPHysics, an open-source code developed based on the SPH method, is used to map the urban flood. However, SPH models are generally more computationally demanding than grid-based approaches. Therefore, this code is accelerated by high performance computing and modern graphic processing units (GPUs), and its Lagrangian nature facilitates the tracking of flood particles in the simulation.

For this research, 1 km² of LiDAR data from Montpellier City in France, which is highly prone to flooding, is selected. The city geometry serves as a fixed solid boundary condition, and the dynamic boundary treatment is used to simulate fluid particles. In the SPH method, dynamic particles are fixed on the boundaries. As a fluid particle approaches the solid boundary, the density and pressure of the dynamic particles escalate, leading to an augmentation in the magnitude of the repulsive force acting on the fluid particle. Therefore, the fluid particles are maintained within the domain. The interparticle distance in the SPH simulation is also considered 0.5 meters. By comparing the results, specifically the inundation extent and velocity, with another numerical simulation, the application of the SPH method demonstrates success in simulating floods. This comparison affirms the effectiveness of the SPH method in capturing water flow dynamics. Identifying the flooded areas using the available LiDAR data provides decision-makers with essential information to develop plans addressing urban flood challenges and minimizing their impact.

Multiphysics and data-driven modeling for cardiovascular biomedicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN WALL SHEAR STRESS PREDICTION FROM CONCENTRATION USING A SURFACE TRANSPORT MODEL

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ABSTRACT

Measuring wall shear stress (WSS) is critical for many fluid flow applications, especially in the biomedical and cardiovascular fields. Accurately estimating WSS in vascular flows necessitates detailed velocity field measurements near the vessel walls, which are challenging to obtain experimentally due to inherent noise and limitations in the near-wall resolution. Motivated by concentration measurements in in-vivo CT angiography as well as in-vitro experiments, we hypothesized that such concentration measurements could be used to obtain WSS vectors in a data-driven fashion. The advection-diffusion mass transport equation relates concentration to velocity and WSS could be obtained from near-wall velocity in an inverse modeling framework. However, rather than focusing on inferring 3D velocity fields from 3D concentration data, we employ a surface transport model derived in [1] where the 3D transport equation is projected on the wall and velocity in the advection term is replaced by WSS thanks to its simple relationship with near-wall velocity [2]. Physics-informed neural networks (PINN) are used to solve the inverse problem and infer the WSS vector field from the near-wall concentration data. In this study, we used multiphysics computational fluid dynamics (CFD) simulations (Navier-Stokes equation and advection-diffusion transport) to obtain synthetic concentration measurement data. Idealized stenosed geometries were used to test the model. As a proof-of-concept, we focused on an idealized stenosed channel geometry to simplify the projection of the equation onto the surface (remove the curvature terms). We demonstrate the success and limitations of this approach in estimating WSS topology and WSS magnitude. Our streamlined inverse modeling process involved solving just one reduced-order surface equation rather than solving the traditional set of equations (continuity, momentum, and mass transport) in 3D and is therefore computationally very efficient.

Acknowledgement: This work was funded by NSF grant No. 2205265.

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Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT OF A SCALABLE HIGH-PEFORMANCE PARTICLE SOLVER WITH MULTI-RESOLUTION BACKGROUND CELLS PRECONDITIONING IN GPU

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ABSTRACT

Incompressible fluid analysis using the ISPH, which is one of the particle simulation models, requires solving the pressure Poisson equations. The linear equation solver using the iterative method such as the conjugate gradient (CG) method takes up most of the time-consuming part in the ISPH calculations. In addition, the number of iterations in the linear equation solver may increase as the simulation model scales. This is a common problem not only in particle methods but also in the implicit time iteration methods of the other discretized computational models. It is known that in FDM, FEM, etc., high quality preconditioning such as geometric multigrid preconditioning can greatly improve the convergence property of iterative methods, but there are few applications of the latter in particle methods. In this study, we developed a framework of geometric multigrid preconditioner using background cells to accelerate the solution procedure of the pressure Poisson equation in the ISPH, and implemented it in GPU environments. We demonstrated the effectiveness of cell-based multigrid preconditioner for a simple dam-break problem and for the tsunami run-up problem to the Fukushima Daiichi Nuclear Power Plant with complicated geometries of structures. As a result, the proposed method marked 3.64 times speedup over the CG method without preconditioning for a simple dam-break problem with 10 million particles. The tsunami run-up simulation was performed for about 8.15 million particles. The simulation with the CG method without preconditioning took 45 hours, whereas the same simulation with the proposed method took only 23 hours. Through this numerical experiment, we show that the proposed method is also effective for practical complex flow problems.

Advanced multiscale and adaptive numerical methods for non-linear solids
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BEAM-TO-COLUMN ADHESIVELY-BONDED CONNECTION: A MECHANICAL MODELIZATION

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ABSTRACT

This paper presents two simple analytical expressions to predict the strength and stiffness of an adhesive beam-to-column connection between glass pultruded profiles (GFRP) subjected to shear and bending loads (vertical load applied at the free end of the beam). The joint configuration is characterized by a tubular column made of a commercially available hollow profile with a square cross section and two U-profiles arranged in the form of a built-up beam. The mechanical behaviour of this type of connection is governed by shear and bending stresses acting on the beam, with the latter becoming torsional stresses inside the adhesive layers and responsible for the failure of the connection.

Regarding the strength prediction, a simple mechanical model based on the scheme of a single lap joint subjected to a traction force is presented. While, for the stiffness prediction, a simple formula for evaluating the adhesive layer deformability is proposed. With the latter, and by means of the Principle of the Virtual Power, the vertical displacement (corresponding to the vertical load applied) is evaluated and, consequently, the stiffness of the joint predicted.

A comparison with the experimental results available in current literature has made it possible to verify the effectiveness of the proposed formulations which involve relatively few geometrical and mechanical parameters.

Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SCALABLE DIFFERENTIABLE CFD LIBRARY FOR SCIENTIFIC MACHINE LEARNING

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ABSTRACT

The integration of High-Performance Computing (HPC) and Machine Learning (ML) in Computational Fluid Dynamics (CFD) faces hurdles due to the reliance on low-level programming languages for HPC solver development. These languages often lack native differentiability and streamlined support for ML, creating a disconnect that hinders the development of high-performance ML-integrated simulation frameworks. The XLB library [1], utilizing the Lattice Boltzmann Method (LBM), is engineered to overcome these barriers, offering a tool that unites computational efficiency with ML advancements.

By leveraging recent compiler technologies from the AI community (like JAX, Pallas, and Warp), XLB, written entirely in Python, implements a highly extensible CFD package based on the Lattice Boltzmann method that elegantly blends high performance with ML capabilities. From the HPC perspective, XLB is capable of scaling on distributed multi-GPU systems, and leveraging cutting-edge hardware features to enable efficient out-of-core computation in the Grace-Hopper Nvidia architecture.

XLB's LBM kernels are fully differentiable, allowing seamless integration with ML libraries such as JAX. This capability is exemplified by its practical applications in fluid mechanics, which include deep learning correctors to reduce simulation errors and leveraging ML techniques for advanced fluid flow control.

The library's design not only facilitates the convergence of HPC and ML in CFD but also does so with an emphasis on accessibility and performance.

XLB is publicly available at: https://github.com/Autodesk/XLB

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Immersed-boundary variational methods: Theory, data structures, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NONLINEAR SOLID MECHANICS WITH THE SHIFTED BOUNDARY METHOD

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ABSTRACT

We propose a new unfitted/immersed computational framework for nonlinear solid mechanics, which bypasses the complexities associated with the generation of CAD representations and subsequent body-fitted meshing. This approach allows to speedup the cycle of design and analysis in complex geometry and requires relatively simple computer graphics representations of the surface geometries to be simulated, such as the Standard Tessellation Language (STL format). Complex data structures and integration on cut elements are avoided by means of an approximate boundary representation and a modification (shifting) of the boundary conditions to maintainoptimal accuracy. An extensive set of computational experiments in two and three dimensions is included.
Performed under the auspices of the U.S. Department of Energy under Contract DE-AC52-07NA27344 (LLNL-ABS-857519).

A SIMULATION FRAMEWORK FOR THERMOPLASTIC COMPOSITE CONTINUOUS RESISTANCE WELDING OF STRUCTURAL AEROSPACE JOINTS

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ABSTRACT

Thermoplastic composite welding is a promising manufacturing technique to join aerospace components as the need to design more structurally efficient aircraft increases [1]. Previously limited to coupon laboratory samples or small static (spot) welding applications, a new technique has been proposed for continuous operation to mitigate power and consolidation force demands [2]. Using a robotically controlled welding apparatus a local zone is heated, in this case with an electrically resistive implant, which then moves along the joint. A candidate example for the continuous welding process is an aircraft fuselage skin and stringer assembly.

In any bonding process, the interface properties of the joint between the two adherends is unobservable or would be invasive to inspect in real-time. Additionally, the potential for geometry, boundaries, or materials to change along the weld path complicates production assessment of joint strength. Computational analysis is therefore used to create a virtual twin of the weld to calculate an accurate prediction of thermal history and determine optimal input conditions for power, speed, and pressure. Using a process simulation framework to systematically define the welding parameters allows for coupled implementation of a multi-physics hierarchy to extend functionality of the digital twin to include electrical behaviour, melting of the thermoplastic matrix, and subsequent flow compaction and solidification. The culmination of this modelling capability leads to a prediction of bond consolidation and residual stress, which in turn will affect mechanical performance in service. The over-arching goal of this simulation framework is to gain confidence in the welding operation, reduce costs associated with production inspections or testing, and implement real-time control, whilst ensuring that the resulting joint satisfies the original performance requirements.

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Architected materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DESIGN OF TRANSIENT HEAT MANIPULATORS VIA ISOGEOMETRIC OPTIMISATION

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ABSTRACT

Heat manipulators are devices in which arrangement of materials with significantly different thermal conductivities is carefully designed to create a certain effect: e.g. to concentrate heat flux in some area (heat concentrator) or create an illusion that the heat map resembles some target heat distribution (thermal cloak, thermal inverter, etc). In this work, we use level-set isogeometric topology optimisation to design such heat manipulators for transient heat flow. The NURBS basis functions are used to parameterise geometry, topology and unknown temperature. Control points in the topology parameterisation serve as design variables, and the optimisation is carried out with the Sequential Quadratic Programming algorithm. Isogeometric analysis is used to solve the state and adjoint boundary value problems.

Performance of the method is demonstrated on a several benchmark examples.

Advances in computational mechanics for flow-induced vibrations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EVALUATING FLOW-ADDED DAMPING VIA LINEAR STABILITY ANALYSIS

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ABSTRACT

Hydroelectric turbine designers require knowledge of the damping coefficient of a turbine blade to assess its durability under cyclic loading. In the case of hydraulic turbine, the flow-added damping is dominant. Numerical evaluation of flow-added damping is challenging with current methods which involve complex and computationally expensive simulations that require moving meshes like one-way or two-way coupling fluid structure interaction simulations. We introduce a new, efficient, and fast approach for assessing the added damping coefficient of a cantilever plate. This method is based on a finite element formulation using the FreeFEM ++ solver. The weak formulation of the problem is implemented in the solver and the flow-added damping is then evaluated through linear stability analysis. The method is quick to setup as the mesh is fixed. The computation time is a few minutes compared to several hours for existing methods. This method will eventually allow us to consider complex geometries, to get closer to a realistic turbine design. Our ultimate objective is to use an existing CFD flow solution on a guide vane or a runner blade and perform the linear stability analysis about it.

Keywords: Flow-added damping, Finite element method, Linear stability analysis, Hydraulic turbines, Hydrofoils

Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BAND GAP EVOLUTION IN NONLINEAR DYNAMICS OF METAMATERIALS MADE STRUCTURES VIA GRADUALLY-CHANGING MECHANICAL PROPERTIES

Riccardo Augello[*1] and Erasmo Carrera*[1]

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ABSTRACT

Metamaterials stand out as they diverge from the properties found in nature, offering unparalleled control over the propagation of waves, both in electromagnetic and acoustic fields. In contrast to conventional materials, which are limited by natural properties and exhibit predictable behaviors, metamaterials provide the unique ability for designers to tailor-made responses to specific inputs. The band gap is crucial in determining how metamaterials interact with and control waves, offering exceptional opportunities for tailoring their behavior in a range of applications.

An essential part of designing the band gaps and structural behavior of metamaterials is the numerical simulation. Traditional methods usually depend on three-dimensional (3D) and two-dimensional (2D) simulations, which are often hindered by high computational expenses and significant nonlinear approximations, respectively. The solution presented in this study involves the application of the Carrera Unified Formulation (CUF) [1]. CUF brings two significant advancements ideal for metamaterials analysis: the capability to represent them efficiently using a singular one-dimensional (1D) beam model, and the incorporation of the complete Green-Lagrange strain tensor. The first innovation addresses the typical constraints of standard finite element methods, significantly reducing the computational cost associated with solid finite elements and surpassing the limitations of both 2D and 1D models. The second key feature effectively overcomes nonlinear assumptions, particularly in scenarios involving von K´arm´an nonlinearities, as for 2D elements. Moreover, the proposed approach allows for the implementation of any nonlinear assumption, to evaluate the accuracy and reliability of the different theories.

The research delves into the examination of thin-walled structures and metamaterials, placing a strong emphasis on the alteration of band gap characteristics as these materials undergo significant displacement and the influence of the chaning of mechanical properties. This study extends to include a comprehensive nonlinear analysis, integrating the complete Green-Lagrange strain equations, which is critical for accurately assessing the behavior of these materials. Practical examples are provided to illustrate the evolution and development of band gaps in these structures. A key aspect of this research is the comparison of results obtained from this comprehensive approach with those derived from von K´arm´an approximations. This comparative analysis underlines the enhanced accuracy and relevance of incorporating full Green-Lagrange strains in understanding the dynamic properties of thin-walled and metamaterial structures.

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Computational modeling of cardiac fibrosis: A multiscale, multiphysics challenge
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A PHYSIOLOGICALLY VALID, MULTI-PHYSICS MODEL OF THE LEFT ATRIUM TO ASSESS THE INFLUENCE OF FIBROSIS ON ATRIAL FUNCTION

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ABSTRACT

Image-based cardiac electromechanical (EM) models are valuable for understanding cardiac function in both normal and pathological conditions, aiding in diagnosis and therapy planning. Overcoming methodological challenges is crucial for advancing these models. This includes improving computational efficiency and robustness for model personalization and prolonged simulations under diverse conditions. Additionally, achieving physiological completeness with therapy-relevant mechanisms enhances predictive capabilities.

In this talk we focus on left atrial EM and present a modeling framework that integrates a 3D EM model with the physiologically comprehensive 0D CircAdapt model for closed-loop circulation. We show that the model successfully replicates physiological behaviors, responding to alterations in loading conditions and contractility induced by experimental protocols.
We employ this model to simulate fibrotic remodeling in atrial tissue, capturing its impact on electrophysiology, active contraction, and passive elasticity and investigate hemodynamic changes that can lead to thrombosis in the atria.

The framework's mechanistic completeness and efficiency make advanced left atrial EM modeling applications feasible. It enables the exploration of parameter spaces over prolonged periods, crucial for personalized modeling. The model's reliability in predicting acute transient responses to interventions underscores its utility in clinical scenarios.

Deep and machine learning methodology in the context of application to computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ENHANCING MUSIC GENERATIVE SYSTEM THROUGH OPTIMIZATION WITH AI AND MIR TECHNIQUES

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ABSTRACT

With the ongoing evolution of AI techniques, these technologies are actively pursued, resulting in significant achievements across various fields, including music generation. However, the generation process is still undergoing development and faces challenges, particularly in the realm of music. Since music is intangible and aesthetic, research in this area has taken diverse approaches. One significant challenge lies in acquiring data for the training process. Sound, being complex data, is currently captured through spectrum and MIDI data. While MIDI data remains more popular in music generation, limitations persist in obtaining data from musical instruments with and without MIDI systems. To address this, the SoundFont system has been employed to gather data from all sounds for the training process. Nowadays, various AI models, including RNNs, GANs, CNNs, etc., are available. In this study, a type of RNN called LSTM was utilized, with different models investigated for the training process. The current system was further modified using MIR techniques, manipulating audio data by adding feature extraction, such as tempo, velocity, and duration adjustment. The current system's achievement lies in the ability of the Hierarchical LSTM model to generate music from any type of musical instrument. However, an apparent challenge in music generation is finding an optimal approach. Researchers typically use two methods: Subjective and Objective. Both methods are still in development. The current system investigates both approaches, with the subjective method requiring more time due to its reliance on human input through surveys and musician perceptions. In contrast, the objective approach is computational and mathematical. In this research, both methods were examined to assess aesthetic value and computational achievement while seeking an optimal way to generate music. Looking ahead, a new generative system will be created for not only Burmese traditional instruments, not currently involved in the MIDI system but also any traditional instruments. By enhancing music generative systems, numerous benefits can be derived, including the capability to generate all instruments, support for musicians' creativity, and improvement in the music industry.

Novel mathematical and numerical models for multiphysics and multiscale systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING THE IMPACT OF SURFACE TENSION ON LUNG MECHANICS: A CONTINUUM POROMECHANICAL APPROACH

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ABSTRACT

During respiration, lung mechanical response can be explained by the interaction of forces arising at the alveolar walls and the surface tension resulting from the air-liquid interface in the alveoli. This interfacial phenomenon plays a crucial role in respiratory function and has been linked to the hysteresis observed in quasi-static pressure-volume curves. Pulmonary surfactant, a complex mixture of proteins and lipids that is adsorbed, desorbed, and squeezed out from the air-liquid interface, is primarily responsible for the pulmonary hysteretic response, as it dynamically modulates surface tension values [1, 2]. This physicochemical activity of surfactant and the intrinsic porous nature of the lung parenchyma reveals the need to understand lung mechanics from a multiphysics perspective.

Poromechanical models present a unique opportunity to improve the modeling of respiratory mechanics, as they, by construction, couple ventilation with lung deformation. However, modeling the impact of alveolar surface tension on lung response has received less attention than alveolar wall elasticity, possibly due to its complex multi-scale behavior that depends on the physicochemical nature of surfactant activity. Indeed, previous attempts by poromechanics to address lung response only consider the elastic term related to lung tissue in their constitutive modeling framework, offering a fully poroelastic response [3].

In this work, we developed a continuum poromechanical model of lung mechanics suitable for incorporating the impact of surfactant dynamics and the resulting alveolar surface tension on organ response. Following a standard Coleman-Noll procedure, we derived a constitutive relation for lung stress, which includes a collapsing pressure resulting from the surfactant-dependent surface tension. Governing equations were solved using a non-linear finite element scheme on human lung geometries. To test our model, we derived quasi-static pressure-volume curves for air-filled and saline-filled lungs. Remarkably, our model can predict different inflation and deflation pressure-volume limbs, resulting in hysteretic loops. Furthermore, our simulations highlight the role of the surfactant alveolar activity in pulmonary compliance of P-V curves.

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Advances in computational biomechanics and mechanobiology
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IDENTIFICATION OF HYPERELASTICITY IN HUMAN ARTERIES USING A MACHINE LEARNING BASED VIRTUAL FIELDS METHOD

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ABSTRACT

Identification of constitutive properties of tissues is important in biomechanics, as they are needed to simulate some surgical treatments like percutaneous coronary intervention for instance. Due to advances of techniques like digital image correlation (DIC) in experimental mechanics, the virtual field method (VFM) has become a major approach to identify mechanical parameters, which rely upon the availability of full-field displacement data. However, it is limited to a prior-selected classical material model posing challenges, especially for biological materials [1]. Recently, machine learning has become a promising alternative as a nonparametric identification method. In this paper, an approach using a machine learning framework (NN-EUCLID) combined with the VFM is proposed. NN-EUCLID stands for Efficient Unsupervised Constitutive Law Identification and Discovery and is based on a specially designed Neural Network (NN) architecture [2]. The “Unsupervised” means training only requires measurable full-field displacement and reaction force data, whilst the lack of stress labels is compensated by leveraging a physics-motivated loss function. This framework has demonstrated its performance for hyperelasticity using 2D numerical data. Our study focuses on discovering the mechanical behavior of arterial walls in a bulge inflation test by extending the current 2D framework to 3D. To this aim, we combined the NN-EUCLID method with VFM. To be more precise, due to practical challenges in measuring a full-field strain map and distribution of reaction forces by DIC technique in experiments, we firstly adapted the original loss function based on VFM, thanks to its ability in material characterization using DIC on a small region of the inflated artery. Moreover, by designing the different virtual fields, we generated different combinations of tension/shear strain data for the training process, which strengthens the method's robustness with heterogeneous materials. Lastly, we implemented the trained model in Abaqus via a user-defined subroutine to validate our identified tissue properties. We showed that the identified model can accurately predict the mechanical response of the arterial wall in a different loading scenario like biaxial tension, demonstrating the potential of the combined VFM and NN-EUCLID method 3D tissue characterization.
Keywords: Material identification, Neural networks, Virtual field method, Inflation test

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DESIGN FOR MATERIAL PROPERTIES OF ADDITIVELY MANUFACTURED METALS USING TOPOLOGY OPTIMIZATION

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ABSTRACT

Geometrical design rules have been used extensively in topology optimization (TO) with the aim of ensuring the metal additive manufacturability of optimized designs. More recently, TO schemes that integrate the thermal and mechanical state of the part through simplified AM process simulation paved the way for reducing overheating, part distortion and residual stress buildup [1]. It is evident from these studies that the part design (geometrical features) to be realised by AM greatly influences the temperature transients and, hence, the microstructural features, which in turn control mechanical properties such as strength, ductility, and toughness.

In metal Additive Manufacturing (AM), the deposited material is subjected to a series of heating and cooling cycles. The locally occurring temperature peaks and subsequent cooling rates determine an important aspect of the microstructure: solid-state phase fractions and, ultimately, the local material properties. Since the geometry of the part determines the local thermal history during AM, this offers an opportunity to influence material properties through design.

For this purpose, a density-based TO framework is used for the design optimization. The thermal history of the compliance-minimized design is evaluated by a simplified wire arc additive manufacturing (WAAM) process model. The relation between the cooling time and the resultant yield strength is then obtained by an empirically established alloy-specific microstructural response [2]. Within the gradient-based optimising scheme, the sensitivities of the cooling time with respect to design variables were computed with the evaluation of the cooling time spent in the critical temperature range in a continuous and differentiable manner. Numerical examples illustrate the capability of our approach in adapting the design to achieve various strength values within a control volume for high strength low alloy steels, where resulting phase fractions significantly influence mechanical properties.

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Advanced materials: Computational analysis of properties and performance
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A GRADED METAMATERIAL-BASED CUSHION FOR BROADBAND NOISE MITIGATION OF IMPACT-DRIVEN OFFSHORE MONOPILES

Ana Carolina Azevedo Vasconcelos[*1], Dingena Schott[1] and Jovana Jovanova[1]*

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ABSTRACT

The next generation of offshore wind farms will consist of larger wind turbines with higher power capacity. To withstand the upcoming wind turbines into the offshore environment, new foundations with larger sizes are also required. Monopiles are commonly used as wind farms foundations and are installed into the seabed through the blows of an impact hammer. During the pile driving process, the pile wall vibrates, which results in high underwater noise emission in frequency ranges that are harmful to marine life.

Several noise mitigation systems were developed to reduce the underwater noise, especially in frequency ranges around 1000 Hz. However, the increase of monopiles' diameter can also induce high noise emission in frequency ranges lower than 1000 Hz. For the existent noise mitigation systems, the attenuation of low frequency noise is not straightforward, which may require the combination of different systems to attain enough noise reduction.

To efficiently mitigate low frequency noise, acoustic/elastic metamaterials (A/E MMs) have been explored due to their unique properties for vibration control. Such properties rely mainly on the A/E MM microstructure, which are formed by resonant elements. The use of A/E MMs to mitigate the noise from the pile driving process was numerically introduced by [1], where a meta-interface formed by single resonators was designed. The meta-interface showed a noise reduction at a frequency range associated with the fifth vibration mode of the monopile, which was causing the highest noise level. In case the noise caused by other pile modes exceed the limit levels, new resonators should be designed.

This work proposes a new cushion formed by graded spiral resonators that will mitigate the energy coming from distinct monopile's vibration modes. Different from the resonators presented in [1], the spiral type has shown a better vibration attenuation performance in even lower frequency ranges, which can be more suitable for the upcoming monopile designs. In addition to that, a stress analysis is performed to verify the cushion's structural integrity. This is an important design step, since the cushion undergoes several impact hammer blows. Finally, the noise mitigation performance is verified, which shows a reduction of noise in frequency ranges where traditional mitigation systems are not completely efficient. The findings of this work open the doors to the development of new noise mitigation systems that are more indicated for the upcoming impact-driven offshore monopiles.

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Isogeometric methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ASSESSING PERFORMANCE IN SHELL ANALYSIS: A COMPARATIVE STUDY OF ISOGEOMETRIC AND SPECTRAL ELEMENT METHODS

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ABSTRACT

In this contribution, we compare various shell formulations used in isogeometric analysis (IGA) and spectral element method (SEM) analysis of thin-walled structures. Additionally, we compare the results of a newly developed spectral element method based on NURBS-based geometry definition with the aforementioned methods. Different assumptions in the formulations and numerical integration methods are presented, and comparisons are made using well-known obstacle course examples and free-form shells. The performance assessment measures are not limited solely to deformation results but also include shear diagrams and the condition numbers of the stiffness matrix in each method. A discussion about the accuracy of the methods in estimating geometry and their impact on the precision of outcomes is also included. It will be demonstrated that neither the condition number nor the precision of the geometry definition provides sufficient information to predict the performance of the methods. Surprisingly, considering different aspects of shell analysis, the conventional isoparametric SEM exhibits very good performance.

Key Words: Spectral element method, Isogeometric analysis, Shell formulation

DATA-DRIVEN COMPUTATIONAL FRAMEWORK FOR SHELLS

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ABSTRACT

This work proposes a distance-minimizing data-driven framework for large deformation of composite shells. The basic idea is to minimize the distance between the constraint space and the material space of the stress-strain data [1], thus bypassing the need for material modeling. The material space can be derived from numerical simulations, e.g., using the homogenization method, or from experimental tests of real samples. The constraint space contains the equilibrium and compatibility equations derived based on the seven-parameter Büchter-Ramm shell [2] that is suitable for both thin and moderately thick shells. The minimization procedure consists of an iterative operation [3] between the two spaces to find the optimal solution ensuring the minimum distance functional. Some numerical examples of homogeneous and multi-layered shells are investigated to verify the efficiency of the proposed algorithm. An analysis of the data size and accuracy of the proposed model is also discussed.

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USING NONLINEAR DOMAIN DECOMPOSITION METHOD AS A SMOOTHER IN NONLINEAR MULTIGRID

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ABSTRACT

Nonlinear Partial Differential Equations (PDEs) frequently arise in different fields of science, e.g. material science, fluid dynamics etc. Finite element discretization of such problems usually leads to large nonlinear systems, either due to the need of higher accuracy, having to deal with large physical sizes or both. Solution of such big discretized nonlinear problems needs fast, highly scalable, and parallelize solvers. Nonlinear multigrid is a well-known method for efficiently solving nonlinear boundary value problems. The full approximation scheme (FAS) solves nonlinear problems on fine and coarse grids. To smooth the nonlinear problem a nonlinear smoother must be utilized and since implementation is supposed to be in matrix-free form for an efficient finite element code, this form of implementation of the smoother should be plausible. For this purpose, Nonlinear Restricted Additive Schwarz Method (NRASM) seems to be a very interesting choice. The method converges with the same rate as linear iterations applied to the linearised equation. In addition, it is inherently parallel and proper to be implemented in matrix-free form. We combine FAS and a nonlinear restricted additive Schwarz method to obtain hybrid NRASM/FAS. The full approximation scheme is used to solve the nonlinear problem and the NRASM is used to smooth the nonlinear boundary value problem in local subdomains on each level of the multigrid method. Within the NRASM, we use the Jacobian-Free Newton Krylov method as the local solver on each subdomain. We consider different nonlinear equations in three dimensional space as test problems. Several parameters of the methods were investigated in this study to have a better understanding of influence of the parameters on the efficiency of the method, the behavior of the methods and its convergence rate.

Advances in material model calibration for computational solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN EQUATION ERROR APPROACH FOR DIRECT INVERSION FROM FULL-FIELD WAVE DATA

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ABSTRACT

We consider the problem of reconstructing the mechanical properties of soft tissue from full-field wave data. This is a problem of interest in the elastography field where the mechanical properties are used to noninvasively diagnose, and monitor the treatment of various diseases. Standard techniques used to solve this inverse problem either oversimplify the physics of the problem, resulting in poor reconstructions of the mechanical properties, or are too computational expensive to be done in real time. We present an equation error approach that can be used to efficiently solve the inverse problem. We discuss some of the mathematical properties of this variational formulation, and evaluate its performance on simulated data.

Multiphase flow and non-Newtonian fluid - Modelling and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL STUDY OF THE IMPACT OF GROOVES ON REFRIGERANT FLOW BOILING IN MICROCHANNEL HEAT EXCHANGERS

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ABSTRACT

Microchannel heat exchangers are increasingly being adopted due to their compact size and superior heat transfer performance in air conditioning systems. To promote the heat transfer in microchannels, grooves on the inner walls of microchannels are commonly employed, but detailed detailed design of the grooves is inhibited by the lack of visualization of their impact on the flow boiling characteristics inside the channel. In this study, a Volume-Of-Fluid method based CFD simulation of saturated refrigerant flow boiling in microchannels has been developed. Validation of the simulation has been conducted with experimental data for smooth walled rectangular microchannels with the refrigerant R32 for mass flux range of 25-100 kg/m2-s, typical of air conditioning systems. Subsequently, simulations were performed for grooved wall rectangular microchannels. The results show an increase of 57% in heat transfer coefficient between smooth and grooved wall microchannels. Analysis of the simulation results reveals that the grooves promote heat transfer by increasing the wet area of the wall around the slugs and the elongated bubbles formed as the refrigerant boils in the channel. Furthermore, effects of the different operating conditions including inlet mass flux and wall heat flux on the slug/elongated bubble flow regime shape and behavior along the grooves are discussed. This study aims at demonstrating the potential of numerical simulations for designing microchannels along with complicated structures like grooves.

Imaging-based methods in computational medicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADVANCING LUNG FINITE ELEMENT MODELS THROUGH DIGITAL IMAGE CORRELATION TECHNIQUES

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ABSTRACT

Lung diseases, including chronic obstructive pulmonary disease (COPD), asthma, and most recently, COVID-19, pose a significant threat to global health, with over 4 million deaths worldwide and billions of dollars spent annually [1]. Computational models play a crucial role in advancing therapies and deepening our comprehension of lung physiology, yet pulmonary biomechanics research on this frontier remains notably absent; these endeavors are hindered by the lack of mechanical experiments needed to inform and validate models. Recently, we developed a custom-designed electromechanical breathing mimicry apparatus to replicate both artificial and diaphragm breathing [2]. This ventilation system enables testing ex-vivo lungs from various species such as rats, pigs, and even humans. The amalgamation of high spatial and temporal local meso-scale tissue strains and displacements collected continuously via digital image correlation (DIC) innovatively interfaced with global macro-scale pressure-volume lung loading facilitates a wealth of unprecedented data acquisition. Building on our established reduced-order modeling framework of a porcine lung specimen [3], the present study focuses on advancing this pipeline to create the first structurally-representative three-dimensional model of the breathing human lung. This inverse finite element model incorporates key features of the lungs, including the intricate structure and material properties of the airways, the pleura, and the parenchyma. Pressure is applied directly to the parenchymal tissue of terminal airways, employing a poroelastic formulation. Strains, pressure, and volumes obtained experimentally from the ventilation apparatus are utilized to calibrate the model. While the current human lung model employs generalized thoracic geometry, ongoing objectives focus on harnessing topological whole lobe morphology using 3D scanning techniques to enable patient-specific pipelines; thus far, this proof-of-concept has been promising when applied to our study of rat lungs. This work represents pioneering applications of experimental-to-computational lung research pipelines; the results underscore simulation efficiency and paves the way for developing more sophisticated models, which provide fresh insights into lung function, and contribute to the broader field of computational biomechanics.

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Data-driven methods for modeling complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

WALL-MODELS OF TURBULENT FLOWS VIA SCIENTIFIC MULTI-AGENT REINFORCEMENT LEARNING

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ABSTRACT

The predictive capabilities of turbulent flow simulations, critical for aerodynamic design and weather prediction, hinge on the choice of turbulence models. The abundance of data from experiments and simulations and the advent of machine learning have provided a boost to turbulence modeling efforts. However, simulations of turbulent flows remain hindered by the inability of heuristics and supervised learning to model the near-wall dynamics. We address this challenge by introducing scientific multi-agent reinforcement learning (SciMARL) for the discovery of wall models for large-eddy simulations (LES). In SciMARL, discretization points act also as cooperating agents that learn to supply the LES closure model. The agents self-learn using limited data and generalize to higher Reynolds numbers in reproducing key flow quantities. We test the discovered wall model to canonical flat plate boundary layers, which shows good predictable capabilities outside the Reynolds numbers used to train the model.

Machine learning and multiscale modeling for complex materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FROM INITIAL PHASE SEPARATION TO SELF-ASSEMBLY IN BLOCK COPOLYMER THIN FILMS

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ABSTRACT

Block Copolymers (BCPs) are a class of self-assembly materials. Due to chemical incompatibility between constituent blocks, while annealed, BCPs evolve from the as-cast state into lamellae, cylinders, and more depending on chain makeup. BCP chains experiences chemical incompatibility, segregate, and then gradually self-assemble into such morphologies. BCP chains in this process are not permanently stuck with a single morphological object, but likely travel around to get associated with different morphological objects. In order for BCP chains to do so, they have to jump over the matrix phase or overcome the energy barrier induced by microphase separation. Even at the equilibrium state, BCP chains are observed to keep hopping around and be engaged with multiple morphological objects, while the whole BCPs hold the overall equilibrium morphology.
Understanding of how BCP chains travel across the matrix phase to join another morphological object may give rise to enhanced long-range ordering; thus, we here study the trajectory of BCP chains when they hop and quantify the energy barrier they experience and should overcome. We use a molecular dynamics model we previously developed based on a Kremer-Grest model [1, 2, 3], where we explored a multidimensional parameter space associated with BCP ordering by adopting a machine leaning approach – an autonomous loop using a Gaussan Process control algorithm interatively selects high-value simulations to compute. With this established model, we build a BCP film on a substrate with periodic boundary conditions imposed along the plane and form vertical morphologies (cylinders and lamellae) because vertical morphologies make much easier for us to keep track of BCP chains. In the fully equilibrated morphologies, we carefully choose a single BCP chain that is part of a cylinder or a sheet of lamella. The selected BCP chain is displaced by a fraction of the repeat spacing each step with translation disabled and rotation allowed. Each displacement is followed by energy minimization and annealing, and this process is carried out until the selected BCP chain completely travel across the matrix phase. The thermodynamic integration is then preformed using the displacement and the force the molecule experiences every step to compute the free energy.

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GAS EFFECTS ON HORIZONTAL RIBBON GROWTH OF SILICON

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ABSTRACT

Horizontal ribbon growth (HRG) of silicon wafers for solar cells is a promising method of growth from melt. HRG can significantly reduce the production cost and waste compared to Czochralski method where there are significant losses due to squaring and sawing of cylindrical ingots produced. Although, production of silicon sheets has been demonstrated using HRG, producing uniform and thin sheets has proven formidable. In HRG of silicon, the sheet floats on its melt due to its lower density and is pulled horizontally. The heat of fusion is removed by a cold impinging helium jet.

In this study, a three-phase computational model of HRG was developed including the moving solid-melt and melt-gas interfaces, solidification kinetics, and the physics of the triple-phase line (TPL) where the three phases meet. For spatial discretization, an hp-finite element method was utilized with fourth-degree basis functions on triangular elements, which was stabilized using a streamline upwind Petrov-Galerkin approach that allows the same order used for pressure and velocity. Furthermore, an arbitrary Lagrangian-Eulerian moving mesh and local mesh adaptation were employed.

Three-phase (solid, melt, and gas) and two-phase (solid and melt) models of horizontal ribbon growth were compared to identify the significance of different gas effects. The boundary conditions at the melt-gas and solid-gas interfaces for two-phase simulations were obtained from decoupled simulations of the gas phase. The results showed that the gas shear stress strongly changes the flow and temperature fields and the position of the triple-phase line. Also, the gas pressure distribution determined the vertical position of the triple-phase line. In the absence of growth angle effects, the results of the two-phase simulation with convective heat transfer coefficient, shear stress, and pressure specified closely matched that of the three-phase model. Even with non-zero growth angle effects, the two-phase model with all the boundary conditions applied agreed well with three-phase simulation results despite increased deviations at higher pull speeds. Finally, the results indicated that gas-induced velocities are significant compared to the Marangoni and buoyancy velocities, which could lead to flow instabilities and the variations in solid shape as observed in HRG experiments.

Constitutive modeling of complex materials with machine learning and artificial intelligence
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NEURAL ADDITIVE METHOD ACCELERATED DISCOVERY OF MATERIAL SYMMETRIES FOR HYPERELASTIC MATERIALS

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ABSTRACT

Biological and human-made systems, including biological tissues and metamaterials for soft robots, often leverage specific forms of anisotropy to achieve optimal performance with minimal costs. The varieties of anisotropy can be captured through structural tensors or eigenprojection. This talk presents an approach in which we leverage the expressivity of the neural network to capture the precise behaviors of anisotropic hyperelastic materials while introducing feature space suitable for symbolic regression to enhance the trade-off among the predictive and descriptive accuracies, the interpretability, and the simplicity of the learned model. In this divide-and-conquer method, we start by acquiring a separable representation of the polyconvex hyperelastic energy functional using univariate neural networks. A key advantage of this step is its scalability concerning the number of strain invariants input into the energy functional, which can often exceed five for certain materials. In the subsequent phase, we employ genetic programming to perform symbolic regression on each of the learned univariate neural networks. This process transforms the neural network models into concise symbolic equations. Compared to the generic symbolic regression modeling effort, the success rate of training of this paradigm is higher, as demonstrated in the numerical experiments. Compared to the neural network models, the learned symbolic models often express the mathematical expression more economically than the neural network parametrization. This efficiency leads to the elimination of arithmetic operations and makes the computations more efficient without excessive pruning and fine-tuning.

Physics-informed machine learning for numerical modelling in engineering and science
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTATIONAL MECHANICS ENHANCED BY PHYSICS AND DEEP LEARNING

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ABSTRACT

Computational modelling is one of the most important ways to study challenging mechanics problems. During modelling, numerical techniques are leveraged to approximate solutions of physics partial differential equations (PDEs), such as equilibrium equations and conservation of momentum. In recent years, deep learning has emerged as a promising tool for solving PDEs [1-3]. Therefore, the deep learning-based computational mechanics field has gained increasing attention. In this work, a computational framework enriched by physics and deep learning is proposed for nonlinear solid mechanics problems. In the proposed framework, the displacement is constructed by neural networks with radial basis function, while the solving process is done by minimizing the energy functional of mechanics systems. Numerical examples, including the 2D Cook's membrane and the 3D twisting rubber cases, are conducted to show its remarkable performance and stability. It has been demonstrated that the proposed framework is locking-free and compatible with parallel computing schemes. Consequently, the proposed framework provides an effective way for nonlinear solid mechanics with great potential.

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Data science and machine learning applications for composite materials and biomedical engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT OF AN ELASTIC DEFORMATION ATLAS OF CEREBRAL MAJOR ARTERIES VIA STATISTIC APPROACH

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ABSTRACT

Medical literature suggests that the potential cause of aneurysmal pathology may be attributed to the interaction between the biomechanical characteristics of arterial walls and hemodynamic factors, including wall shear stress and pressure. Research indicates that in cases where vascular structures exhibit specific characteristics or patterns, there is a likelihood of corresponding patterns of aberrant blood flow, and such scenarios may elevate the risk of arterial vascular diseases[1].

Nowadays, statistical methodologies are gaining prominence in vascular morphology research. Data-driven studies, leveraging extensive blood flow simulations, seek to elucidate the pathogenesis of vascular diseases through a systematic analysis of the relationship between blood flow patterns and vascular variability. In this study, we employed unsupervised learning techniques to develop a Deformation Atlas for Cerebral Major Artery (CMA), utilizing a publicly available dataset of cerebral vasculature. This atlas is presented in a spatial coordinate format, depicting the distribution and range of variation in shapes of non-diseased CMA.
We applied Principal component analysis (PCA) for curves[2] to identify essential components that contribute to geometric variability and calculated their probability distributions. This analysis focused on how these distributions affect the vascular geometric parameters, contribute to the vascular classification, and influence blood flow patterns.

To mitigate the impact of nuisance parameters in shape data, such as minor misalignments and re-parameterizations, we employed Elastic Shape Models (ESM) which provides a Riemannian framework that is invariant to affine transformations and re-parameterizations of contours[3]. This enables the handling of data derived from different sampling methodologies and various discretization approaches in spatial coordinates, ensuring consistent analysis across diverse cases. We demonstrated the application of EMS in processing centerlines derived from medical images of varying resolutions (test data). We computed the probability density of these test datasets, which facilitated the categorization of the centerlines based on their shapes. This method illustrated how these centerlines were deformed from a baseline shape, providing insights into the morphological variations observable in the medical imagery.

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Transport phenomena in micro/nanofluids
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VARIATIONAL MULTISCALE MOMENT METHODS FOR THE BOLTZMANN EQUATION

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ABSTRACT

The Boltzmann transport equation yields conservation equations for mass, momentum and energy from its first five moments. These equations require closure relations for the deviatoric stress and heat flux so as to balance the number of unknowns with the number of equations. The most storied closure method is the Chapman-Enskog expansion[1] which yields a sequence of closures in orders of Knudsen number: Euler's and Navier-Stokes-Fourier equations at zeroth and first order, Burnett equations at second order and so on. Unfortunately, the Burnett equations are known to be unstable[2].

In this presentation, we propose a new framework for deriving closure relations based on the Variational Multiscale (VMS) method[3], which was originally created to derive stabilized Galerkin formulations to advective PDEs. Our VMS closure process subsumes the Chapman-Enskog expansion while opening the door to novel closures. It also provides a criterion based off the entropy production inequality of the Boltzmann equation for assessing the quality of a given closure.

Focusing on the linearized Boltzmann equation, we will describe the VMS framework and use it to introduce an entropy stable extension to the Navier-Stokes-Fourier equations. We will then present results on the application of these equations to the stationary heat transfer problem and the Poisseuille channel problem. In both setups, we obtain solutions that are accurate far beyond the early transition regime of rarefied gas flow that they are designed for.

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Data-driven methods for modeling complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN DISCOVERY OF QUANTITIES OF INTEREST AND THEIR GOVERNING EQUATIONS IN COMPLEX SYSTEMS

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ABSTRACT

We tackle two common challenges in discovering interpretable physics from data of complex systems: 1) the identification of physics-informed quantities of interest and 2) the discovery of interpretable dynamics from incomplete measurements. We propose two approaches that constrain deep learning optimizers to identify physically-meaningful variables. This aims to merge the highly effective yet opaque feature learning of deep networks with the straightforward interpretability of physical laws. I will demonstrate the use of deep delay double-encoders to recover full-state variables and their governing differential equations from partial measurements, with applications to chaotic systems and uncertainty quantification.

Mechanobiology of cells, vesicles and biomembranes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THEORETICAL AND COMPUTATIONAL MODELLING OF CELL-CELL ADHESION IN 3D

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ABSTRACT

Cell-cell adhesion and decohesion are important in biology, to keep cellular tissues together and, in addition, to allow disengagement of cells during remodeling. Due to the fluid nature of the surface of the animal cells, the molecular bonds that keep cells together are laterally mobile. It limits the application of classical theories of adhesion and interfacial fracture in this context. These molecular bonds form clusters, attach to the cytoskeleton through mechanosensitive adapter protein molecules, and undergo turnover by endocytosis. Cells can tune various properties of these molecular bonds including diffusivity, stiffness, and force sensitivity. We lack a fundamental understanding of how mechanics, chemistry, and biological regulation integrate to support the adaptable function of cell-cell adhesion, and how effective mechanical properties of adhesions such as strength and toughness depend on the molecular properties of bonds. We develop a mathematical and computational model for cell-cell adhesion, based upon Onsager's principle, coupling active gel models of actomyosin cortex (which take into account shape changes, myosin activity, viscous dissipation, and the turnover of the cortex) to the adhesion dynamics of mobile binders (which take into account bond formation and dissociation kinetics, force sensitivity, and bond mobility) that would allow us to understand how the actin cortex and the adhesion complexes work together to give rise to adaptable junctions. For computational analysis in full three-dimensional generality, we consider an ALE parametrization based on an offset to represent the fluid deformable cell surface and use the Local Monge Parametrizations (LMP) method to approximate tensor fields on general surfaces given by a collection of local parametrizations using a FEM setup based on subdivision surfaces. Our work provides a conceptual background to guide new experiments that probe cell-cell adhesion and decohesion. We show how the interplay of mechanics and chemistry at adhesion patches leads to a wide range of behaviors that cells can use to stabilize cell-cell junctions during physiological stretch or to selectively detach during morphogenesis.

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Modeling mechanics of materials with voids
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MECHANICS OF NETWORK GLASSES: GENERATION, DEFORMATION, ELEMENTARY EVENTS AND THEIR PREDICTION

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ABSTRACT

A fundamental understanding of the mechanics of glasses remains an ongoing challenge in research, and is highly relevant to society and industry. This contribution focuses on the mechanics of glasses with topological structures of covalent bonds, leading to rings, i.e., nanovoids, of various shapes and sizes. A typical example of such material is silica glass, consisting of the most abundant elements on this planet.

The first part of this contribution presents two novel strategies to generate network glasses: the melting-quenching technique and a dual Monte Carlo bond-switching algorithm. While the first approach may be seen as the rather classical strategy to numerically generate glasses on the nanoscale, the second approach is a non-classical method that consists of a sequence of topological flip transformations in an initially hexagonal lattice.

The second part of this contribution focuses on mimicking the mechanical response behavior of such disordered materials on a molecular level. To do so, we use an overdamped, athermal description, which is particularly beneficial in disentangling the complex deformation mechanics of glasses. We also comprehensively discuss the theory of the mechanics of disordered materials. This method allows one to disentangle elementary fracture events in the network materials and study the anomalous yielding behavior of silica glass, which can be linked to the appearance or disappearance of nanovoids. Furthermore, this method allows one to study the problems of prediction and reversibility.

The third part of this contribution builds on the assumption that zones prone to experiencing nanovoids during deformation are predefined in the material and can be identified in the material prior to any deformation approach. Thus, we apply a local scanning method that can generate prediction fields, presenting spots prone to rearrangements. It is shown that these spots do indeed reveal a high correlation with the actual localized fracture events in the material due to mechanical deformation.

MODEL ENRICHMENTS IN REDUCED ABLATION MODELS FOR HYPERSONIC FLIGHT SIMULATION

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ABSTRACT

During hypersonic flight, air reacts with a planetary entry vehicle's thermal protection system (TPS), creating reaction products that deplete the TPS. Reliable assessment of TPS performance depends on accurate ablation models. New finite-rate gas-surface chemistry models are advancing state-of-the-art in TPS ablation modeling, but model reductions that neglect chemical species may be necessary in some cases for computational tractability. This work develops a theory-informed stochastic enrichment operator to improve the predictive capability and quantify uncertainties in such reduced models while maintaining computational tractability. We focus on a high-fidelity air-carbon finite-rate model [1] in which a low-fidelity model only tracks a subset of chemical species in the high-fidelity model. Discrepancies in predicted carbon monoxide production result. We propose an enrichment operator, embedded in the low-fidelity model, to quantify the effect of neglected species. The enriched model is calibrated with Bayesian inference and validated with posterior predictive assessments. Numerical results show the enrichment operator improves the low-fidelity model's predictions without significantly increasing computational cost.

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Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A GENERALIZED FRACTURE MECHANICS-BASED MODELING METHOD FOR PREDICTING BEHAVIORS OF SHORT AND LONG FATIGUE CRACK PROPAGATION

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ABSTRACT

Failures due to high cycle fatigue (HCF) are characterized by the progression of short cracks across different length scales. This progression includes initial crack formation (nucleation), the growth of short cracks, and the subsequent extension into longer cracks. The sequential development of cracks across scales ultimately leads to fatigue failure. Given that most structural components exhibit predominantly short cracks within the HCF range, the behavior of long cracks holds lesser significance. Attempts have been made to bridge the mechanics of short and long crack propagation by exploring concepts such as crack closure [1] and a two-parameter mechanical driving force incorporating the influence of crack tip plasticity [2]. Despite some successes, existing fatigue crack growth models have lacked a comprehensive mechanical approach to adequately capture the intricate behavior of short cracks, thus limiting their practical applications. In light of recent studies conducted by the author's group on crack propagation modeling [3-4], a new generalized crack growth model has been proposed. This model aims to predict the behavior of both short and long cracks by considering two driving force parameters, Kmax and ΔK, affected by cyclic plastic deformation (i.e. residual stress fields), along with corresponding crack growth thresholds, ΔKth and Kmax,th influenced by the crack length in the short crack regime. This approach enables a unified modeling of fatigue crack behavior across short and long crack regimes. Fatigue crack growth datasets of titanium and aluminum alloys e.g. Ti-6Al-4V titanium and 7075-T6, 2024-T3 aluminum alloys were employed to validate the accuracy of the proposed model. Predicted results demonstrate a strong agreement with experimental crack growth data for these materials, affirming the efficacy of the proposed model.

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Verification techniques in computational physics and applied mathematics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VERIFICATION OF THE HIGH-ORDER VLASOV CODE LOKI IN THE RELATIVISTIC REGIME.

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ABSTRACT

Kinetic simulation of plasmas using grid-based codes is inherently costly due to the high-dimensional setting of the problem. The kinetic code LOKI implements finite difference algorithms in a variety of configurations up to 3D-3P. High-order accurate algorithms (4th and 6th order) are used as a way to mitigate the high cost of simulation by reducing the requisite number of grid points required for a given level of accuracy. This talk discusses various verification strategies that have been employed in LOKI in the relativistic setting for both Vlasov-Maxwell and Vlasov-Poisson. Manufactured solutions are used to verify the expected convergence behavior of the numerical methods in settings near to their operational use. Exact solutions for physically relevant problems, such as Landau damping, are further used to probe code performance.

ACCELERATING DYNAMIC FLUID SOLVERS IN FLUID-STRUCTURE INTERACTION SIMULATIONS

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ABSTRACT

The computational complexity inherent in fluid-structure interaction (FSI) simulations requires the development of efficient methods for solving both fluid and solid dynamics. This is especially crucial in minimizing the computational cost associated with fluid flow, given that it typically constitutes the most resource-intensive aspect. This need has driven the building of Reduced order models (ROMs) capable of predicting both steady-state and dynamic fluid flow. Currently, there exists frameworks where deep learning-based ROMs are used to accelerate steady-state solvers. Quite recently, a successful endeavor has utilized neural operators to expedite the solution of steady-state Partial Differential Equations (PDEs). Extending such framework to dynamic problems is demanding; it requires the management of the coupling between the ROM and the numerical solver at each time step, which poses a challenge. Moreover, one must carefully decide the input length, output length and how frequently the numerical solver should be called to prevent error accumulation while using the ROM prediction. Also, approaches such as those involving differentiable hybrid neural models rely on automatic differentiation (AD), limiting integration with non-AD-supported Computational Fluid Dynamics (CFD) or FSI platforms. In this study, we present a novel approach for accelerating the dynamic fluid solver by building a framework that allows the flexibility of using the ROM prediction as an initial guess of the fluid solver at any chosen time-step. Careful consideration of the prediction length and frequency of usage of the ROM output as initial guess prevents error accumulation while expediting solver convergence. Moreover, we develop a purely data-driven deep learning-based ROM, eliminating the need for the numerical solver to support AD. The capability of the method is verified by testing it on various dynamic fluid benchmark cases where the ROM prediction is used to accelerate fluid flow cases at Reynolds numbers (both interpolative and extrapolative) not encountered during the training of the ROM. For all cases, the methodology significantly speeds up the CFD solver while preserving the dynamical behavior of the flow and satisfying the conservation laws. The results obtained show the potential of applying the methodology to much complex cases as well as other computational fields that involve similar dynamics or the solution of time dependent PDEs.

Modeling mechanics of materials with voids
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ENHANCED MECHANICAL BEHAVIOR OF NICKEL-COATED GRAPHENE GRAPHENE REINFORCED COCRFEMNNI NANOLAYERED COMPOSITES

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ABSTRACT

High entropy alloys (HEAs) especially CoCrFeMnNi HEAs have drawn more and more attention due to their excellent combination performance. However, the mechanical properties of archetypal CoCrFeMnNi HEAs still remain to be improved due to the single-phase FCC crystal structure. Although many efforts have been made on strengthening methods by grain refinement [1] or nitriding [2], the improvement of the mechanical properties is still unsatisfactory. To improve the mechanical properties of CoCrFeMnNi HEAs and broaden their application fields, we proposed that adding functionalized graphene in CoCrFeMnNi HEAs and investigated nanoscale mechanical properties and the strengthening mechanism using molecular dynamics (MD) simulation in this paper. The mechanical properties of pristine single-layer graphene nanoplatelets (GNPs) and double-side nickel-coated GNP (Ni-GNP-Ni) reinforced CoCrFeMnNi composites (Ni-GNP-Ni/CoCrFeMnNi) are studied under uniaxial tension by molecular dynamics (MD) simulations. Meanwhile, their tensile properties are also compared with those of double-side nickel-coated GNP with vacancy defects (Ni-defected GNP-Ni) and double-side nickel-coated multilayer GNPs (Ni-nGNPs-Ni) reinforced CoCrFeMnNi-based nanolayered composites. The simulated results show that the mechanical properties of Ni-GNP-Ni /CoCrFeMnNi composites are improved significantly by the addition of Ni coated GNPs. With increasing of the layers or volume fractions of GNPs in Ni-nGNPs-Ni, the elastic modulus, tensile strength and fracture strain of the composites are all increased significantly, but there exist a critical layer thickness between two graphene layers for Hall–Petch and inverse Hall–Petch relations of nanolayered composites. It is concluded that the main strengthening mechanisms for Ni-GNP-Ni/CoCrFeMnNi composites are strong interface bonding, effective load transfer from the CoCrFeMnNi matrix to the Ni-GNP-Ni and dislocation/twin strengthening by analysis of the evolution of atomic structure.

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Mesh-free particle methods for multi-physics problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL INVESTIGATION ON FLUID-FLEXIBLE-STRUCTURE INTERACTION BASED ON SPH METHOD

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ABSTRACT

The fluid-flexible-structure interaction (FFSI) is characterized by the large deformation, the thin structure and the complex of the flow field. Accurately simulating FFSI poses three challenges, which are the reproduce of thin structure, the capture of moving interface, and the numerical stability of multi-physics field coupling, respectively. In this study, the FFSI is simulated by the smoothed particle hydrodynamics (SPH) because of its nature advantage in dealing with the moving interface. The shell model with single-layer particles[1] is introduced into SPH to simulate the thin flexible structure. The truncation error caused by single-layer boundary is modified by the normal flux approach[2]. κ-ε turbulence model[3] is introduced into SPH to enhance the numerical stability and capture complex flow details. In addition, other techniques or models that ensure efficiency and stability of the calculation are used in this study, including PST (particle shifting technique), δ-SPH method, and GPU (graphics processing unit). The flows around the single filament are simulated to verify the accuracy and stability of current FFSI algorithm based on the SPH method. Several important parameters that affect the motion characteristics of filaments are discussed to reveal the flow mechanism.

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Multiphase flow and non-Newtonian fluid - Modelling and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE IMPACT OF ADVECTIVE DISPERSION ON THE DISPLACEMENT FLOW OF TWO HERSCHEL-BULKLEY FLUIDS IN A CONFINED GEOMETRY: EXTENDING THE D2DGA MODEL FOR NON-NEWTONIAN FLUIDS

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ABSTRACT

Complete removal of drilling muds and sealing the space between formation and steel casing with cement slurries are the key elements in successful construction of water, geothermal, oil, and waste storage wells. This process is called primary cementing and the foremost purpose of this process is to eliminate gas leakages, which occur when the cement layers become inefficient in sealing the gap space. The primary cementing operation includes the invasion of a viscoplastic fluid at a high Peclet number (Pe≥10^5) into an eccentric annulus filled initially with another viscoplastic fluid, where the displacing fluid penetrates ahead in the center of the channel. Since the gap distance is smaller than the other length scales, the two-dimensional gap-averaged (2DGA) model is commonly applied to analyze the displacement process [1]. While the 2DGA model is effective in understanding the qualitative behaviours of fluids in confined geometries, it becomes incapable of monitoring the influence of the advective dispersion on the displacement process due to a homogeneous concentration profile considered across the gap [1]. Fortunately, there is another approach, the dispersive two-dimensional gap-averaged model (D2DGA), which is a promising model to capture advective dispersion effects [2]. This model is generated for two Newtonian fluids by modifying the two-dimensional gap averaged (2DGA) model. The key difference between the D2DGA and the 2DGA approaches comes from a 2-layer flow assumption considered for the distributions of fluids across the gap distance. To adapt the D2DGA model for two Herschel-Bulkley fluids, we consider the Augmented Lagrangian method to obtain a weak solution of the governing equations but keeping the same 2-layer flow assumption as the D2DGA model. Although the presence of a plug region in viscoplastic fluids leads to a more uniform front compared with Newtonian fluids, a comparison between the 2DGA model with the D2DGA model for two Herschel-Buckley fluids highlights the ability of the D2DGA model to track the advective dispersion.

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Advanced discretization schemes and solution strategies for computational structural dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A HIGH-ORDER FLUX RECONSTRUCTION APPROACH FOR HYPERBOLIC ELASTICITY

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ABSTRACT

A wide range of loading conditions in solid mechanics are either unsteady or transient, such as cyclical loading or vibration of turbomachinery components, stress concentrations in impulsively loaded homogeneous or heterogeneous materials, and free vibration of complex structures, amongst many others. These require accurate, efficient, and stable space-time discretization of the governing unsteady elasticity equations. While, classical approaches, such as the Finite Element Method (FEM), are widely-used for steady state or spectral vibration analysis, they are less suitable for more general or transient unsteady problems due to the structure of their large globally-coupled mass matrices.

In the current work we adapt the Flux Reconstruction (FR) approach, widely used in fluid mechanics, for the arbitrarily high-order accurate solution of hyperbolic elasticity problems. Similar to classical FEM, FR uses a polynomial representation of the solution in the computational domain. However, unlike FEM, the polynomials in the FR approach have compact support, meaning they are contained entirely within their respective elements. This allows FR to support discontinuous solutions at the interfaces between elements, which in turn reduces their mass matrices to a block diagonal structure, trivial to invert. Importantly this also enables them to maintain arbitrarily high-order accuracy for problems with discontinuous physics, such as step changes in material properties.

Specific focus will be given to development of the aforementioned numerical framework, upwind-based stabilization techniques, verification, validation, demonstration of the benefits of higher-order polynomial representations, and a comparison of different implicit and explicit time stepping approaches. It is expected that the proposed approach will greatly accelerate the solution of hyperbolic elasticity problems, which will be demonstrated via a range of practical example problems.

Geometric mechanics formulations and structure-preserving discretizations for continuum mechanics and kinetic models
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A SELF-CONSISTENT, HAMILTONIAN MODEL OF THE PONDEROMOTIVE FORCE AND ITS STRUCTURE PRESERVING DISCRETIZATION

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ABSTRACT

A large number of interactions between matter and the electromagnetic field may be adequately captured by approximate models which reduce the interaction to a nonlinear polarization of the medium. In many ways, this concept is the heart of nonlinear optics, but also bears relevance in plasma physics in which asymptotic approximations often induce field dependent polarization and magnetization of the electromagnetic fields. A well-known laser-plasma interaction model gives rise to a nonlinear polarization of the electromagnetic medium. In the presence of an inhomogeneous oscillatory electric field, charged particles experience a net force, averaged over the oscillatory timescale, known as the ponderomotive force. Starting from the two-fluid equations, we derive a Hamiltonian model in which the nonlinear ponderomotive force self-consistently couples Maxwell's equations to an acoustic wave-type equation. We call the system of equations so derived the ponderomotive Maxwell system. One finds a simple Poisson bracket for the ponderomotive Maxwell system: it is a direct sum of the Poisson brackets for Maxwell and acoustic wave equations, as well as a coupling bracket.

Because the Poisson bracket is field-free, i.e. the Poisson bivector lacks field dependence, a structure preserving discretization is easily accomplished using finite element exterior calculus (FEEC). We explore the behavior of discretizations based on not only a traditional spectral element FEEC approach, but also a discontinuous broken-FEEC approach. Temporal discretization is accomplished using Hamiltonian splitting. Using both conforming and broken-FEEC methods with both low and high order discretizations in space and time, we simulate the ponderomotive Maxwell system in order to better understand the properties of this new approach to discretizing Maxwell's equations in nonlinear media. In all cases, we find good conservation of energy to the order of the splitting method used, and conservation Casimir invariants (e.g. Gauss's laws) to machine precision. To our knowledge this is the first time-domain solver for Maxwell's equations in nonlinear media which conserves energy and Gauss's laws, accommodates high order discretizations in both space and time, and which may use local, discontinuous basis functions to localize nonlinear solves (allowing for parallel implementation). Moreover, the methods used to discretize the ponderomotive Maxwell system shows promise to generalize well to a broad class of nonlinear wave models. Hence, the favorable qualities found in this solver for the ponderomotive Maxwell system might be used to study a much broader class of models in nonlinear optics and plasma physics.

Next-generation numerical methods for coupled multiphysics problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ROBUST AND SCALABLE SOLVERS IN NONLINEAR POROELASTICITY

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ABSTRACT

Nonlinear poroelasticity models the flow of a fluid through a complex connected structure within a solid, where the solid is undergoing possibly large deformations. One natural application of this, which is our main target, is that of soft tissue. The porous structure of soft tissue is given mainly by blood circulation, which is in charge of providing oxygen to the tissue itself. The large deformation is instead given in many cases by the natural function of some organs, such as the heart and the lungs, but which is also relevant in other contexts such as brain concussions and muscle activity. The system of equations that characterizes this type of materials presents elements from two very different frameworks: nonlinear elasticity and generalized porous media equations, both extremely challenging topics.

In this talk, we will focus on two topics. The first one is robust discretization techniques for such a system of equations, with focus on a difficulty that we have named the "primal inconsistency", which is related to the presence of higher order derivatives in the primal formulation of the model that yield an inconsistent finite element approximation. The second topic will be the development of scalable algorithms for the solution of these equations, which we will base on an extension of the well-known fixed-stress solver for the Newton iterations of a nonlinear solution procedure. We will validate our claims with several numerical tests.

Applications of shape optimization in complex engineering problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MATERIAL AND SHAPE OPTIMIZATION FOR THE ACTIVE RESPONSE OF LIQUID CRYSTAL ELASTOMERS

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ABSTRACT

Liquid crystal elastomers (LCEs) are responsive materials that can undergo large reversible deformations upon exposure to external stimuli, such as changes in temperature. These materials have drawn increasing interest in a wide range of applications, including soft robotics and sensors. While experimental measurements can provide valuable insights into their behavior, computational analysis is essential to exploit their full potential. Accurate simulation is not, however, the end goal; rather it is the means to their optimal design. Such design optimization problems are best solved with nonlinear programming algorithms that require gradients, i.e., sensitivities, of functions with respect to the design parameters, to efficiently traverse the design space. In this work, we design LCE structures using state-of-the-arts shape and material optimization, wherein the material optimization component pertains designing the alignment of the liquid crystals in the elastomeric matrix. To achieve this, a nonlinear LCE model implemented in a scalable and flexible finite element-based open-source framework, namely Serac, performs the analyses. The graph-based Livermore Design Optimization code, LiDO, is used to link the design parameterizations, finite element analysis, and optimization solver, and automate the sensitivity analysis. LCE design problems that optimize both the material orientation and shape to either reach a target deformation or maximize energy absorption are solved.

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Key Words: shape optimization, parameter free optimization, liquid crystal elastomers, nonlinear design optimization, combined shape and material optimization

Computational fluid dynamics (CFD) and fluid-structure interaction (CFSI): Methods and Applications
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AN INTEGRATED FLUID STRUCTURE INTERACTION (FSI) - IMAGE ANALYSIS (IA) TO REVEAL ENERGY ABSORPTION CAPABILITY OF THE HUMAN MENISCUS

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ABSTRACT

The meniscus, characterised by high through-thickness graded porosity, can be seen as a natural hydraulic damper. Energy dissipation experimental tests and macroscopic simulation (FE) on both native architectures (obtained by high resolution micro computed tomography) and artificially generated 3D printed architectures (based on CFD simulations of native tissue architectures) show an increase of energy dissipation by a factor of 100 with respect to common automotive hydraulic dampers (per unit volume of material).
Here we shed light on the mechanisms of energy dissipation at the pore scale by running Fluid Structure Interaction (FSI) simulations in highly deformable fully saturated soft tissues. We couple mesh-based methods for solid deformation and meshless CFD methods for fluid flow. Our investigation introduces a novel methodology that integrates FSI with advanced imaging techniques, providing unprecedented insight into the fluid dynamics of this complex tissue under physiological loading conditions.

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New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFECT OF DISCRETE AND CONTINUOUS SOIL CONTACT IN THE TOPOLOGY OPTIMIZATION OF LARGE-SCALE STRUCTURES

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ABSTRACT

The behavior of large-scale structures is strongly affected by their interaction with their foundation and supporting soil. This vouches for the importance of taking this effect into account when designing these structures. This paper explores the effect of foundation and soil flexibility in the design of structures via topology optimization. We consider the case of discrete contact, in which the structure is supported by pile groups, which are then responsible for transferring the borne load to their surrounding soil, as well as the case of continuous contact, in which the structure is in direct contact with the soil surface. The discrete contact case is modeled using classical finite elements to model the structure, together with the impedance matrix method to model the pile group. Direct continuity and equilibrium conditions at the interface between the structure and the pile group are establish to describe the coupling. Topology optimization is obtained using the Bi-directional Evolutionary Structural Optimization (BESO) method under various boundary conditions, with the goal of minimizing the compliance of the piled structure under a prescribed volume restriction. The continuous contact case is modeled via a coupling of the Indirect Boundary Element Method (IBEM) to model soil response and the Finite Element Method (FEM) to model the supported structure. Topology optimization is obtained using the Topology Optimization of Binary Structures (TOBS) method, to minimize structural compliance under volume constraints. Both analyses consider the case of a tall tower under vertical and horizontal loads, and the case of bridges under external loads. The results from both studies show that soil and foundation flexibility strongly affect the achievable optimization goal and cause the optimization algorithm to find significantly different optimal topologies, when compared to a first approximation considering rigid support for the structures.

Scientific deep learning
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GRAPH NEURAL NETWORKS FOR INTERPRETABLE MESH-BASED SURROGATE MODELING WITH ERROR TAGGING

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ABSTRACT

This work introduces an interpretable fine-tuning strategy for mesh-based modeling in the graph neural network (GNN) framework with application to fluid dynamics forecasting. Given a pre-trained baseline surrogate model, the end result is a fine-tuned model that identifies structures in physical space (corresponding to sub-graphs) intrinsically linked to the forecasting task, while retaining baseline predictive capability. These structures are adaptively produced in the forward pass and serve as explainable links between the baseline model architecture, the optimization goal, and known problem-specific physics. Additionally, through a regularization procedure, fine-tuned GNNs can also be used to identify, during inference, graph nodes that correspond to a majority of the anticipated forecasting error, adding a novel interpretable error-tagging capability to baseline models [1]. Ultimately, the objective is to show how augmenting pre-trained baseline GNNs with trainable adaptive pooling modules results in an interpretable fine-tuning framework for mesh-based predictive modeling. The core elements and contributions of this work are as follows:

(1) Multiscale message passing: Graph neural networks leverage multiscale message passing layers as backbones to model the evolution of an unstructured turbulent fluid flow [2].
(2) Interpretable fine-tuning: A trainable graph pooling layer -- which relies on a learnable node subsampling procedure -- is attached to the baseline GNN, creating an augmented GNN architecture with enhanced interpretability properties. Fine-tuning is then accomplished by freezing the parameters of the baseline GNN and ensuring the parameters in the newly introduced module are freely trainable.
(3) Error tagging: A regularization term, representing a mean-squared error budget, is added to the objective function during the fine-tuning process. The minimization of this term ensures that the fine-tuned GNN tags, during inference, a subset of the graph nodes that are expected to contribute most significantly to the GNN forecasting error, providing an novel avenue for a-posteriori error tagging for mesh-based models.

Demonstrations are performed using unstructured fluid flow data sourced from a backward-facing step configuration at high Reynolds numbers.

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Data-driven methods for modeling complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICS-INFORMED DIFFUSION MODELS: INTRODUCING PHYSICS INTO DATA-DRIVEN PROBABILISTIC MODELS

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ABSTRACT

Denoising diffusion models, a popular class of generative models, have demonstrated exceptional capabilities in matching intricate probability distributions [1]. Their utility has extended beyond the realm of generating authentic-looking images and videos and now also plays an important role in the natural and engineering sciences, particularly in solving inverse design problems, such as designing metamaterials with nonlinear characteristics [2].

Centuries of research have led to a deep understanding of the equations governing such systems. Nevertheless, such generative models are typically still trained to solely match a data distribution, where the data is generated via a forward simulator such as the finite element method. While these data points naturally obey the physics, the model itself has no direct knowledge of the underlying equations.

We introduce a novel framework that integrates physical laws into the probabilistic setup of denoising diffusion models in a consistent manner. This enhances the model's capability to generate more realistic samples by not only adhering to the data distribution but also by respecting the underlying physics. We discuss extensions of this method to incorporate inequality constraints and optimization goals. Our various numerical studies showcase the benefits of incorporating this additional knowledge in training such models.

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Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LOADING DEVICES AND NON-CLASSICAL THERMOMECHANICAL BOUNDARY CONDITIONS

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ABSTRACT

To study thermomechanical deformations of a body B we regard the collection of other bodies contacting B as a loading device L. Here we consider only an intimate loading device defined as one that is perfectly bonded to the boundary ∂B of B and express the action of L on B at points of ∂B as boundary conditions. For simplicity, we first separately study the mechanical and the thermal problems. For the mechanical (thermal) problem, these are expressed as surface tractions (heat flux) at a point of ∂B in terms of displacements (temperature) and their in-surface gradients at points of ∂B. Note that neither surface tractions nor the heat flux, respectively, involve derivatives of displacements and the temperature along the normal to ∂B. For an intimate loading device surface tractions, the heat flux, the displacements and the temperature are continuous across ∂B enabling one to express surface tractions (heat flux) as functional of displacements (temperature) and their in-surface gradients. The leading term for the mechanical and the thermal problem is, respectively, the familiar equation for the Winkler foundation and the Robin boundary condition. Thus, the problem of analyzing the interaction between B and L is reduced to that of delineating deformations of B. The challenging task of showing that this procedure provides deformations of interior points of B close in some sense to those deduced by analyzing the two-body problem is left for a future study.
Boundary-value problems involving non-classical boundary conditions proposed here have not been studied. It is not clear what space of functions to use for the trial solutions since derivatives appearing in the boundary conditions may be higher than those in equations governing deformations at interior points of B. These boundary conditions involve a length scale that may alleviate the dependence of a numerical solution by the finite element method.
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Numerical modelling of composite materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFECT OF MOISTURE ON PROCESS INDUCED DEFORMATION IN CARBON FIBER COMPOSITES

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ABSTRACT

Process induced deformation describes the phenomenon where the dimensions of a manufactured composite part are different from the tooling dimension. One of the key uncertainties in the models that predict process induced deformation is the effect of moisture absorption. The overall behavior of moisture transport in composites is commonly approximated by Fick's law of diffusion despite the absorbed moisture in a composite having both physical (reversible) and chemical (non-reversible) effects on the matrix [1]. Moisture swelling of the matrix will directly affect the composite residual strain and stress state, even absent plasticization, or other degradation effects. Since the full saturation of a part usually requires months to years in a moisturizing environment, the approach typically taken for design purposes is to assume a worst-case moisture content (a fully saturated part), as this is considered to be a conservative approach [2].

This presentation explores the effect of both symmetric and asymmetric moisture gradients on process induced deformation. A Fickian diffusion model was developed in ABAQUS to predict the concentration profiles as a function of time for various L-shape samples. A thermal analogy was then used for the 3D stress analysis in ABAQUS as the equations for thermal strain (1), ε_T, and moisture strain (2), ε_M, are identical:

$$\varepsilon_T = \alpha \Delta T \quad (1)$$
$$\varepsilon_M = \beta \Delta c \quad (2)$$

For the thermal strain, α is the coefficient of thermal expansion and ΔT is the temperature gradient. For the moisture strain, β is the coefficient of moisture expansion, and Δc is the concentration gradient. Inputting concentration profiles as temperature profiles and replacing the thermal expansion coefficient with the moisture expansion coefficient allows for the calculation of deformed part geometries which can be compared to experimental results. During the experiments, it was found that transient moisture gradients with asymmetric concentration profiles caused significantly more spring-in than the fully saturated steady state conditions, implying that the worse-case scenario for the moisture swelling effect is not the fully saturated part. The developed models not only show agreement with the experimental results, but also provide insight into the contribution from in-plane and through-thickness effects.

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Physics-informed machine learning for numerical modelling in engineering and science
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICS INFORMED MACHINE LEARNING-BASED COMPUTATIONAL FRAMEWORK TO ANALYSE NONLINEAR AND HETEROGENOUS VARIATIONS OF PLANT-BASED FOOD DRYING

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ABSTRACT

Computational modelling plays a critical role in investigating the drying kinetics of plant-based foods to achieve energy-efficient drying and produce high-quality dried food products. However, traditional computational methods, such as mesh-based Finite Element Analysis (FEA) and mesh-free particle-based methods, face inherent challenges. Mesh-based FEA encounters significant difficulties when modelling multiphase interactions and the large deformation of materials. On the other hand, mesh-free methods are not very effective in simulating attributes like time-domain variations, and there is a shortage of model developments designed to capture heat and mass transfer variations within the context of food drying. None of the traditional computational approaches have demonstrated the ability to incorporate the inconsistency of material properties in the spatiotemporal domain and heterogeneous conditions when simulating the microscale physical models of plant-based food materials during drying [1]. This study introduces a novel Physics-Informed Machine Learning (PIML) framework to overcome some of the challenges faced by traditional modelling frameworks. The flexibility of this novel framework, coupled with a mesh-free approach, provides various advantages in the context of food drying. It can extract information from both data and physics [1], strengthening the prediction capabilities if one side is weak. If the PIML model is trained with only physics, without labelled data, it can be used to solve physics models [2]. PINN's mesh-free nature and gradient-descent optimization features provide more flexibility to solve nonlinear variations. Furthermore, interface calculations are much easier, allowing for domain decomposition to introduce heterogeneous boundary conditions and property variations easily, making the model more realistic [3].

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Space-time modeling of coupled problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SPACE-TIME FINITE ELEMENT GEOMETRIC MULTIGRID SOLVER FOR FULLY DYNAMIC POROELASTICITY

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ABSTRACT

Constructing higher order numerical methods to coupled systems of partial differential equations, maintaining stability and inheriting most of the rich structure of the continuous problem, becomes increasingly difficult. Space-time finite element methods (STFEMs) allow the natural construction of higher order approaches even to complex systems. STFEMs offer the potential to achieve accurate predictions on computationally feasible grids with a minimum of numerical costs. The iterative solution of the arising algebraic systems requires advanced and tailored techniques. Geometric Multigrid (GMG) Methods are known as the most efficient iterative methods for the solution of large linear systems emerging from the discretization of partial differential equations [M. Anselmann, M. Bause, A geometric multigrid method for space-time finite element discretizations of the Navier–Stokes equations and its application to 3d flow simulation, ACM Trans. Math. Softw., 49 (2023), Article No.: 5, pp. 1-25].

We present and analyze higher order STFEMs for three- and multi-field simulation of poroelastic wave propagation studied, for instance, in computational subsurface or biomedical engineering or seismology and modeled by a coupled hyperbolic-parabolic system [M. Anselmann, M. Bause, N. Margenberg, P. Shamko, An energy-efficient GMRES-Multigrid solver for space-time finite element computation of dynamic poro- and thermoelasticity, Comput. Mech., submitted (2023), pp. 1-30; arXiv:2303.06742]. In the multi-field approach [M. Bause, S. Franz, Structure preserving discontinuous Galerkin approximation of a hyperbolic-parabolic system, Electron. Trans. Numer. Anal., submitted (2023), pp. 1–24; arXiv:2311.01264], the equations are rewritten as a first-order in space and time system such that Picard’s abstract solution theory for evolutionary problems becomes applicable. Families of continuous and discontinuous Galerkin FEMs in space and time are investigated and evaluated. To solve the algebraic systems with complex block structure, GMG preconditioning with local Vanka-type smoothers of GMRES iterations is suggested. The numerical and parallel performance of the approaches are benchmarked for challenging three-dimensional test problems.

Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TAYLOR-SERIES EXPANSION FOR MESHFREE METHODS IN COMPUTATIONAL SOLID MECHANICS

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ABSTRACT

Numerical quadrature based on Taylor-series expansion approaches was introduced in the mid-80s for FEM to develop a parameter-free approach for hourglass control. It laid dormant for a while, and, much later, in the mid 2010s, it resurfaced in the context of RKPM to develop a so-called Natural Stabilization approach, which is arguably the most important recent breakthrough in RKPM that brought the necessary added robustness for a wide range of nonlinear solid mechanics applications. In this talk, I will present a general framework of Taylor-expansion-based methods in computational solid mechanics and its broad applicability to meshfree methods and beyond. I will demonstrate: i. How to develop Taylor-series-expansion-based formulations that are accurate and stable for nearly incompressible deformations; ii. How to stabilize correspondence-based Peridynamics without resorting to costly bond-associated approaches; and iii. How to develop general-purpose large-deformation meshfree thin shells.

Numerical modeling of granular and multiphase flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENTS IN THE USE OF THE BONDED PARTICLE MODEL TO STUDY ORE FRACTURE

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ABSTRACT

In mineral processing, ore breakage is an essential first step for which the objective is to increase the exposed surface area of the valuable mineral, thereby increasing the likelihood of liberation in subsequent separation stages. This process is well known to be energy-intensive, and increasing scrutiny around sustainable practices has heightened the need to examine the efficiency of current practices. Factors such as pre-existing cracks and mineralogical structure are known to affect ore breakage mechanisms. However, isolating and investigating individual factors under experimental conditions is challenging and typically impractical.

Numerical techniques such as the Bonded Particle Model-Discrete Element Method (BPM-DEM) have been developed as a means of investigating in isolation, the effects of different factors on ore breakage behaviour under closely controlled breakage conditions using synthetic rock specimens. In this work, a model is developed to relate microstructural model parameters to the macroscopic mechanical properties that are typically obtained from standard geotechnical breakage experiments. The robustness of the model is evaluated by considering the sensitivity of fracture measures to the variation of model resolution, size-dependency and macroscopic mechanical properties (Young’s modulus and uniaxial compressive strength) of the numerical specimens.

It demonstrated that the macroscopic measures of fracture are in agreement with existing theoretical knowledge, in that the fracture starts with the initiation of stress at the point of contact, initiation of cracks following the accumulation of strain energy exceeding the particle strength, and the progression of cracks through the particle leading to failure. It is further shown that under different configurations, failure occurs with a variable degree of breakage, highlighting the opportunity of using this computational approach to study specific cases toward identifying efficient modes of breakage.

Fluid dynamics and SciML: Navigating challenges and seizing opportunities
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOWARD DISCRETIZATION-CONSISTENT CLOSURE SCHEMES FOR LARGE EDDY SIMULATION USING REINFORCEMENT LEARNING

Andrea Beck[*1] and Marius Kurz*[1]

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ABSTRACT

With a few exceptions, Large Eddy Simulation (LES) methods intended for practical engineering applications are based on an implicit scale separation filter, sometimes also referred to as a grid or discretization filter. For this approach, the induced filter kernel, and thus the closure terms, are determined by the properties of the grid and the discretization operator, leading to additional computational subgrid contributions to the closure terms that are generally unknown in a priori analysis [1].

Our talk will present a novel method for developing discretization-consistent closure schemes for implicitly filtered LES. In this approach, the task of adapting the coefficients of LES closure models is framed as a Markov decision process and solved in an a posteriori manner with Reinforcement Learning (RL) [2]. This optimization framework is applied to both explicit and implicit closure models. The explicit model is based on an element-local eddy viscosity model. The optimized model is found to adapt its induced viscosity within discontinuous Galerkin (DG) methods to homogenize the dissipation within an element. For the implicit modeling, RL is applied to identify an optimal blending strategy for a hybrid DG and Finite Volume (FV) scheme. The resulting optimized discretization yields more accurate results in LES than either the pure DG or FV method and renders itself as a viable modeling ansatz that could initiate a novel class of high-order schemes for compressible turbulence by combining turbulence modeling with shock capturing in a single framework. All newly derived models achieve accurate results that either match or outperform traditional models for different discretizations and resolutions. Overall, the results demonstrate that the proposed RL optimization can provide discretization-consistent closures that could reduce the uncertainty in implicitly filtered LES [3].

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Advanced numerical methods for the modeling and optimization of coupled dynamical systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CALCULATION OF THE FORCED RESPONSE OF A PARTICLE-DAMPED STRUCTURE BASED ON MECHANICAL IMPEDANCE OBTAINED FROM MEASUREMENTS

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ABSTRACT

Mechanical structures optimized for their total weight in particular are often susceptible to vibrations due to low structural damping. In order to dampen vibrations over a broad frequency band, particle dampers are a low cost and effective solution. Energy dissipation is achieved by friction and impacts of the particles inside the cavity. Depending on the excitation level, the behavior of the damper can be described using the solid, fluid or gaseous domain.

Although particle dampers are excellent for reducing vibrations, they are not widely used due to their complex design process. One of the reasons for this is the large number of design parameters. The current state of research involves time-discrete simulation of the individual particles, whereby the calculation time quickly reaches an unacceptable limit as the number of particles increases.
In this work, an alternative approach is proposed to simplify and accelerate the design process. The properties of a given particle container are determined experimentally in form of its mechanical impedance, independent of the system to be damped. As in electrical engineering, the impedance is a complex variable whose phase angle in this case results from the difference angle between the displacement and the force. To determine the mechanical impedance, the damper is excited with a defined displacement amplitude and frequency and the resulting force is measured. An equivalent mass and equivalent damping are calculated from the data obtained and the results are stored in a lookup table.

A beam structure is used to demonstrate the proposed approach. Harmonic balance is applied which is a state of the art method for steady state vibration analysis of nonlinear systems. As the impedance is defined already in the frequency domain, it can be directly used in a harmonic balance framework to obtain the nonlinear forced response function.

The major advantage of this approach is that as soon as the mechanical impedance of the particle damper is known, its effect on the system to be damped can be calculated with low computational effort. This allows for parameter studies to quickly find the optimum position of the damper on the structure or variations of it, as the damper remains independent of the structure itself.

Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SEMI-ANALYTICAL FAILURE PREDICTION OF ADHESIVE JOINTS BY FINITE FRACTURE MECHANICS

Thomas Methfessel[1], *Cherine El Yaakoubi-Mesbah*[1] *and Wilfried Becker**[1]

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ABSTRACT

In many cases adhesive bonding is a very advantageous way to join load-carrying components, in particular when these components are relatively thin. A typical field of application is lightweight construction, where typically two relatively thin sheet-like adherends are joined through an intermediate adhesive layer. This joining technique has the advantage that no screws or rivets are necessary and that the load transfer is distributed over a larger overlapping area. The actual load transfer behavior, however, is somewhat demanding. Due to the given overlap geometry and the generally dissimilar stiffness properties of the adherends and the adhesive, local stress concentrations occur at the edges of the joints, which may trigger the onset of debonding cracks and subsequent failure and in this way determines the effective strength of the given adhesive joints.
The current contribution suggests a semi-analytical structural model for an adhesive joint with a closed-form higher-order description of the adhesive layer and the potential occurrence of a debonding crack. This enables a highly efficient failure prediction by the concept of Finite Fracture Mechanics [1], employing a coupled failure criterion that consists of a stress and an energy subcriterion. The comparison with accompanying finite element calculations and experimental findings reveals the high predictive quality of this approach.

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PHYSICS-CONSTRAINED GAUSSIAN PROCESS VARIATIONAL AUTOENCODER

Thomas Beckers[*1]*

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ABSTRACT

Understanding the dynamics of an observed object and being able to predict its future states is paramount for controlling autonomous systems or robots that interact with their environment. However, learning dynamics from real-world observations is challenging. Variational autoencoders (VAEs) have been one of the most popular approaches to the unsupervised learning of complex distributions. Their effectiveness has been proven in several examples, such as learning handwritten digits and faces, among others. In recent years, VAEs have been extended to process sequential data, such as video clips, by introducing a temporal constraint on the dynamics of the latent space. Thus, using image sequences of a complex system as input data, the encoder may be used to learn a reduced model of an object's dynamics in the video without ground truth data (unsupervised learning). Even though the object's dynamics is typically based on first principles, this prior knowledge is often ignored in the existing literature.

In this presentation, we present our work on a physics-enhanced variational autoencoder that places a physics-constrained Gaussian process prior on the latent dynamics to improve the efficiency of the variational autoencoder and to ensure physically correct dynamics in the latent space. Instead of directly learning the times series in the latent space, the GP models the unknown latent forces acting on the object, as the underpinning structure of the dynamics of the object might be well known. The physical prior knowledge expressed as linear dynamical system is here reflected by the Green's function and included in the covariance function of the Gaussian process. This novel approach improves the data efficiency of the autoencoder and guarantees a physically correct trajectory of the reduced-order model in the latent space with respect to the known object dynamics. The benefits of the proposed approach are highlighted in a simulation.

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Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SOLVER-FREE REDUCED ORDER HOMOGENIZATION FOR NONLINEAR PERIODIC HETEROGENEOUS MEDIA

Andrew Beel[*1] and Jacob Fish*[1]

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ABSTRACT

Computational homogenization methods, particularly reduced-order methods, are crucial tools for reliable prediction of composite material behavior. Building on the recently developed fine-scale solver-free classical computational homogenization (solver-free CCH) [1], we propose a fine-scale solver-free reduced order homogenization approach (solver-free ROH) that avoids solving the fine-scale equilibrium equations and approximates the phase-average eigenstrains by sampling the fine-scale eigenstrain at a small number of points. The solver-free ROH pre-computes history-dependent eigenstrain influence tensors, identifies suitable sampling points within the unit cell, and chooses sampling point contribution factors based on training data from a small set of CCH simulations. During the online stage of the computation, these pre-computed quantities are used to compute unit cell phase-average strains, eigenstrains, and stresses, which are homogenized to give the corresponding coarse-scale quantities. In this presentation, the proposed solver-free ROH is formulated and verified in the context of small deformation in nonlinear periodic heterogeneous media. First, in the formulation, we review the solver-free CCH procedure for computing eigenstrain influence tensors, devise a sampling point approximation of the phase eigenstrains, and walk through the online stage unit cell computation. Next, we verify the solver-free ROH using loading cases outside the training data set. Finally, we use the proposed method to simulate a multilayer composite plate in three-point bending and open hole tension, demonstrating the method's efficiency and accuracy relative to the CCH [2].

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Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICS-INFORMED SPECTRAL LEARNING TO SIMULATE FLUID FLOW BASED ON DISCRETE HODGE–HELMHOLTZ DECOMPOSITION

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[2]*University of Nottingham*

ABSTRACT

We introduce a Physics-informed Spectral Learning (PiSL) for solving the discrete Hodge–Helmholtz decomposition from limited data through a discrete L2 projection. This computational framework seamlessly integrates supervised and unsupervised learning techniques.

The PiSL framework demonstrates spectral (exponential) convergence, showcasing its efficacy in adaptively constructing a sparse set of Fourier basis functions and their corresponding coefficients. This adaptability is achieved by iteratively addressing a sequence of minimization problems, wherein the set of basis functions is incrementally expanded in a greedy fashion. Notably, the imposition of divergence- and curl-free constraints simplifies into a finite set of linear algebraic equations within the Fourier structure.

The performance of our proposed PiSL method is illustrated through several examples, highlighting its capability to efficiently address the discrete Hodge–Helmholtz decomposition from sparse data to predict fluid flow.

16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics

July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING CELLULAR PHENOMENA AND THEIR IMPACT ON THE ORGAN-SCALE PHYSIOLOGY

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ABSTRACT

Computational modeling and analysis play an important role in bioengineering, particularly in the planning of therapies such as drug-eluting stent placement, and in the design of biomedical devices such as implantable blood pumps. Digital representation of blood flow and associated physiological phenomena has the potential to shorten the design cycle and give the designers important insights into causes of blood damage and suboptimal performance. Nevertheless it is clear that a full bottom up modeling across all scales, starting with molecular one, is not always a practical approach. Depending on the objective of the analysis, one needs to choose the appropriate level of abstraction. In many cases in bioengineering, this involves representing cellular phenomena in the blood stream at the homogenized continuum scale.

We give several examples of recent developments, involving drug propagation and vessel wall growth in case of arterial stents, and red-blood-cell damage and platelet aggregation in case of blood pumps. In order to obtain quantitative blood damage prediction, cumulative tensor-based measures of strain experienced by individual blood cells have been developed; red blood cells under shear are modeled as deforming droplets, and their deformation tracked in an averaged sense.

Complex fluid flows in engineering: Modeling, simulation, and optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FINITE ELEMENT SIMULATION OF COMPLEX FLUIDS AND APPLICATIONS IN MANUFACTURING

Marek Behr[1], Blanca Ferrer Fabón[1] and Felipe González[1]*

[1]*RWTH Aachen University*

ABSTRACT

Many flows of engineering interest involve fluids which are governed by complex constitutive relations. For viscoelastic fluids in particular, the advective nature of the constitutive equation presents a significant numerical challenge. Moreover, the intrinsic coupling of three or more distinct field variables means that multiple compatibility conditions of the inf-sup type must be either satisfied or circumvented. Stabilized formulations of Variational Multi-Scale (VMS) type can provide robustness and accuracy at high Weissenberg numbers. They also allow arbitrary combinations of basis functions, including equal-order interpolations for all fields.

Development of these numerical methods is motivated by challenging applications in production technology, including injection molding and additive manufacturing. We will discuss efforts to reduce costly running-in trials for melt-based processes. Flow of polymer melt as it fills a cavity, or exits the printing nozzle, is often highly influenced by the microstructure of the material and by thermal effects.

Even if modeling and simulation of such production processes still involve many open questions, the computational analysis is advanced enough so that the transition to numerical design can be contemplated. We discuss some typical objective functions, process parametrization approaches, and show sample outcomes of automatic design.

Architected materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPLORING IN-PLANE ELASTIC PROPERTIES AND ENERGY ABSORPTION OF THE BIO-INSPIRED GLASS SPONGE STRUCTURES

Hassan Beigi Rizi[*1], Harold Auradou[1] and Lamine Hattali[1]*

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ABSTRACT

The biological systems have evolved a diverse variety of robust skeletal architectures that can be used as lightweight structures to meet environmental requirements. However, the utilization of bio-inspired structures for energy absorption applications remains less common compared to conventional structures due to the novelty of the bionic approach in this field and limited fabrication capabilities. In this study, first we explored experimentally the in-plane elastic mechanical properties of lattice derived from Euplectella Aspergillum Glass Sponges (EA-sponge). Then, the lattice structure was designed by approximating the architecture of EA-sponge using a fused filament fabrication (FFF) process with thermoplastic Polylactic acid (PLA) filaments. The quasi-static compression test was conducted to study the energy absorption behavior of EA-sponges and compare its geometry to three other 2D square-base lattices with diagonal reinforcement and non-diagonal reinforcement. The results are discussed the effect of the geometrical t/d strut ratio, relative density and diagonal reinforcement or not on the maximization of the energy absorption.

Keywords:
Lattice structures, Fused filament fabrication (FFF), Energy absorption, compression test

Computational modeling of extreme-loading events
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SIMULATING THERMALLY INDUCED STRESSES AND THE RESPONSES TO SUBSEQUENT IMPULSIVE LOADING

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ABSTRACT

Many industries rely on simulations with explicit time integration to resolve the wave motion in solids due to the impulsive loads of impacts or explosions. But oftentimes the performance of the impulsively loaded solid is affected by pre-existing stresses due to prior thermal loading. The development of these thermal stresses is governed by the coupled thermo-mechanical equations. But because thermal conduction is much slower than wave motion, and the periods of thermal-stress development are many orders of magnitude longer than those for which explicit schemes are suitable, simulating the development of thermal stresses is typically done with the unconditionally stable time steps of implicit integration schemes. Simulating both loading events therefore requires transferring the computation from implicit to explicit schemes. Some codes offer both scheme types, and they enable the transfer without exporting the solution from one code and importing it into another. However, finite-element simulations involve many algorithms, and some of them – such as the element formulations and contact algorithms – depend on whether the integration scheme is implicit or explicit. The transfer from one scheme to another is therefore not a straightforward procedure, even within a single code.

This presentation introduces an alternate approach to simulating thermal stresses and subsequent impulsive loading on the same domain, and compares it to the sequential use of implicit and explicit schemes. This approach exploits the observation that the critical stable time step of explicit integration of the energy balance is several orders of magnitude greater than the critical stable time step of explicit integration of the equations of motion, given typical combinations of thermal conductivity, density and bulk modulus. This discrepancy allows scaling of the thermal conductivity to the artificially high value at which the two critical stable time steps are equal. With this scaling, the two explicit schemes simulate thermal-stress development at optimal computational efficiency for explicit integration. The fidelity of this approach depends on several considerations, including the damping of artificial dynamic effects resulting from conductivity scaling. Although this approach requires significantly more time steps than implicit integration, the explicit solution on each step is trivial. The primary benefit of this approach is avoiding the need to employ two different integration schemes, and therefore the need to transfer the computation from an implicit scheme to an explicit one. The implicit and explicit approaches to simulating thermal stresses are compared through sample computations and metrics of their computational efficiencies.

Advance modeling and simulation in complex porous media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN INTEGRATED COMPUTATIONAL FLUID DYNAMICS (CFD) - IMAGE ANALYSIS (CFD-IA) TO STUDY THE FLUID FLOW REGIMES INSIDE THE HUMAN MENISCAL TISSUE

Daniel Bell[*1], Jack Waghorne[1] and Olga Barrera[12]*

[1]*Oxford Brookes University*
[2]*University of Oxford*

ABSTRACT

The meniscus, a porous soft tissue renowned for its load-bearing capabilities and energy absorption properties, remains the subject of profound interest in biomechanics. Through high-resolution micro-computed tomography (μCT) scans, we delve into the intricate mechanisms underlying energy dissipation, implementing a novel methodology merging Computational Fluid Dynamics (CFD) with imaging techniques. Our examination highlights the meniscus's architectural resemblance to a sandwich structure, featuring a rigid outer layer and a pliant internal layer composed of collagen channels. These channels, intricately oriented to guide fluid flow, facilitate deformation and energy dissipation, suggesting a potential for optimised damping systems. Our investigation scrutinises the relationship between architectural characteristics and fluid flow dynamics, a pivotal pursuit for researchers endeavouring to identify biomimetic solutions for tissue replacement. Employing high-resolution 3D μCT scans, we analyse fluid flow patterns within the meniscal architecture across a spectrum of inlet velocities spanning from 0.1 mm/s to 1.6 m/s. Our findings unveil statistical correlations between architectural parameters (e.g., tortuosity, connectivity, porosity, and pore size) and fluid flow dynamics (e.g., number distribution, permeability). Some channels exhibit exceptional Reynold’s number values, reaching 1400 at an inlet velocity of 1.6 m/s, with a discernible transition from Darcy's regime to a non-Darcian regime occurring around an inlet velocity of 0.02 m/s. Furthermore, we identify location-dependent permeability variations ranging from 20 to 32 Darcy. Regression modelling shows relations between fluid velocity and tortuosity at elevated inlet velocities, while channel diameter emerges as a significant factor at lower inlet velocities. Moreover, as inlet velocities escalate, deviations from preferential flow directions increase, resulting in a notable reduction in the concentration parameter by an average of 0.4. This pioneering research offers invaluable insights into the fluid flow dynamics within the meniscus and its intimate interplay with structural attributes. By elucidating these intricate relationships, our findings pave the way for the development of biomimetic solutions tailored for tissue replacement leading to new innovation in biomechanics and regenerative medicine.

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Emerging topology and shape optimization techniques in computational design of materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATION OF TOPOLOGY OPTIMIZATION METHODS TO SPATIAL PACKAGING OF INTERCONNECTED SYSTEMS WITH THERMAL STRESS CONSTRAINTS

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ABSTRACT

Key Words: Spatial Packaging of Interconnected Systems with Physics Interactions, Neural Networks, Multi-Layer Perceptron, Electrothermal System, Finite Element Method

In the current industrial landscape, engineering systems often involve the packaging and routing of the various components. The design of these systems relies heavily on the expertise of engineers. Automated methods have been developed to solve the packing and routing problems independently. Jessee et al. have introduced a framework for 2D Spatial Packaging of Interconnected Systems with Physics Interactions (SPI2) which simultaneously solves the packing and routing problem while considering the implications of the physics interactions within the system [1]. The physics model involved the uncoupled thermofluid analysis of heat generating components connected via fluid-based cooling pipes. This study extends the SPI2 framework to include structural considerations, exploring the effects of thermal expansion of the cooling pipes on the optimal layout. The device locations, pipe widths, and connection points remain as the design parameters for representing the system. A finite element model is developed to analyze the elastic response of the pipes and the design sensitivities are derived using an adjoint analytical method. Support spring elements are introduced to model the fixed boundaries at each component preventing pipe expansion into the components. The design is subject to a constraint on the thermal stresses caused by the repeated cycles of heating and cooling in the pipes. This methods' capability is demonstrated by optimizing three thermal-fluid-structural systems, with results compared to designs obtained from the baseline SPI2 model. The study also explores the application of a Multi-Layer Perceptron for the real-time surrogate modelling of the SPI2 framework [2]. The Multi-Layer Perceptron mechanism learns the spatial topology of the system, mapping the initial input parameters to a system layout with optimized physics-based performance.

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Uncertainty characterization and error control to enable predictive simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SOLVING STOCHASTIC INVERSE PROBLEMS FOR CFD USING DATA-CONSISTENT INVERSION AND AN ADAPTIVE STOCHASTIC COLLOCATION METHOD

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ABSTRACT

The recent development of data-driven approaches has increased interest in developing robust and efficient algorithms to exploit data in engineering design and modelling in CFD. A common set of oberved data d can be some function of a system output, or some desired (targeted) data. A frequent question then arises: what should be the model input that gives as output the targeted or observed data. Solving such inverse problems using a high-fidelity CFD model is very expensive in computational time and storage. This cost is even more important if the CFD model is subject to uncertainties. We are often interested in a model output, defined as a quantity of interest (QoI) whose value, while in presence of uncertainties, will no longer be a scalar but a functional depended on the uncertain parameters. Besides the cost of high-fidelity CFD problems in presence of numerical uncertainties, the model must accurately describe highly nonlinear flow dynamics (like shock waves, etc).

The inverse problem we consider here takes a given model and an observed (targeted) output probability density function (pdf) on QoI, and builds a new model input pdf which is consistent with both the model and the data in the sense that the push-forward of this pdf through the model matches the given observed pdf. We present in this work a non-intrusive adaptive stochastic collocation method [3] coupled with a data-consistent inference framework of [1,2] to efficiently solve stochastic inverse problems in CFD. This adaptive surrogate model is built using a stochastic error estimator as refinement indicator in simplex elements. The efficiency of the proposed method is evaluated on analytical test cases and two CFD configurations. The proposed method is shown to be able to reconstruct both an observed pdf on the data and key components of a data-generating distribution in the uncertain parameter space.

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Verification techniques in computational physics and applied mathematics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VERIFICATION WITH ASYMPTOTIC SOLUTIONS: A NOVEL APPROACH FOR RADIATIVE TRANSFER PROBLEMS

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ABSTRACT

This work proposes to add a new dimension to the method of asymptotic analysis as verification. Conventional employments of this method compare a solution of higher order equations to the appropriate asymptotic limiting solution. The mathematical mechanism of asymptotics can however be invoked to determine the order that the higher order system ought to converge to the lower and verify that a simulation converges at the expected rate, providing greater coverage over the whole parameter space between the two solutions that requires only a solution to the asymptotic equations. In the context of radiation transport, the convergence relationship at the origin from transport to diffusion is found in terms of mean free time, t for infinite medium Green's solution problems to be $O(t^{-3/2})$ for planar geometry and $O(t^{-5/2})$ for spherical. Also, functions are found to represent the error away from the origin as a function of a self similar parameter. Finally, an initial layer correction term for anisotropic initial conditions is derived to bookend the analysis at early and late times. These results are combined into an powerful tool that yields extensive verification analysis with only a single solution of the radiative transfer simulation code.

New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DESIGNING A TRUE WAVE-FOCUSING ACOUSTIC BLACK HOLE THROUGH TOPOLOGY OPTIMIZATION

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ABSTRACT

The acoustic black hole is a device designed so that the wave propagation velocity is gradually reduced, ideally down to zero, at the same time as the amplitude is progressively increased. Thus, in the ideal case, the wave will never reach the end of the device, which has motivated the name ‘black hole’ for it. Such a device can be used to damp incoming waves, for weak signal sensing, and for wave focusing. For transverse elastic waves in beams and plates, such devices have been developed and extensively investigated during the last 20 years. However, the corresponding effect for acoustic waves in fluids has been much less studied. Unfortunately, the few types of layouts that have been suggested in the literature turn out to essentially lack the wave-focusing effect, despite their often-good damping properties. Here we demonstrate that density-based topology optimization can be used to design the interior of a wave guide that exhibits strong broad-band wave focusing. A complicating factor is that viscothermal effects turn out to be significant in this type of device and need to be considered in the optimization. Direct modeling through the linearized, compressible Navier–Stokes equations would be extremely computationally demanding for topology optimization. We therefore model these effects by a generalized impedance boundary condition at solid walls together with the Helmholtz equation in the bulk volume. This boundary condition is potentially present at each element interface in the computational mesh and the corresponding boundary condition is scaled by the square of the jump of the design variable across the interface. Thus, in the limit of zero–one-valued design variables, the viscothermal impedance boundary condition will only be imposed at solid–air interfaces. Using this strategy, we were able to design through topology optimization a truly wave-focusing waveguide device with length 255 mm and radius 115 mm that shows strong wave focusing towards a region at the end of the device in the 400–1000 Hz frequency band. In contrast, the standard type of design for a waveguide acoustic black hole, first suggested by Mironov and Pislyakov (Acoust Phys+ 48(3):347–352, 2002), is a very efficient damping device but fails to provide any wave focusing at all.

Mathematics and algorithms for predictive digital twins (DT)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MULTI-FIDELITY MODEL FOR LARGE-SCALE WAVE ENERGY EXTRACTORS

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ABSTRACT

The primary objective of this study is to efficiently forecast the motion of a floating rigid structure, which embodies a wave energy converter designed to harness the energy of sea waves. We introduce a multi-fidelity model based on domain decomposition. A high-fidelity solver is spatially coupled with a Reduced Order Model (ROM) utilizing Proper Orthogonal Decomposition (POD). The whole (large) computational domain is partitioned into a small computational domain, where the high-fidelity model operates, and the POD basis functions are precomputed for the remaining area along with an overlapping zone.

The high-fidelity model is used in a small computational domain located in the vicinity of the body where the flow exhibits complex nonlinear phenomena (like wave overtopping) that are difficult to model with a linear POD subspace. The utilization of the POD model extends beyond this region for two key reasons. Firstly, we enforce boundary conditions on the small high-fidelity domain using a physical POD subspace rather than resorting to artificial boundary conditions. Secondly, the global POD modes play a dual role by propagating informations across the entire computational domain.

We propose a projection-free reduced-order model where POD temporal coefficients are derived by minimizing the differences between the high-fidelity solution and the POD ansatz in the overlapping zone between high-fidelity and POD domains. Simultaneously, the POD model is tasked with consistently propagating the incoming wave, necessitating the POD ansatz to match some measurements obtained from inflow sensors, such as water elevation. The temporal coefficients of the POD ansatz are thus determined by simultaneously minimizing both quantities.

In this study, POD computation involves snapshots for both velocity and Volume of Fluid (VOF) fields, with the latter numerically representing the air-water interface position. The same temporal coefficients are applied to both velocity and VOF. Typically, sensors give only VOF information, and boundary conditions are enforced for both velocity and VOF.

The dynamics of the floating body are simulated within this framework, resulting in precise predictions of the body's motion for both in-sample scenarios (replicating the same flow configuration as used to compute the POD basis) and out-of-sample scenarios (predicting a flow configuration not included in the POD basis). Subsequently, this model is envisioned for application in numerical simulations of wave energy converter farms, which entail assembling several patches akin to the singular structure presented in this study.

Physical models and reduced order models augmentation with data for physics-informed machine learning in real-world applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THERMODYNAMICS-INFORMED NEURAL NETWORKS FOR SUPER-RESOLUTION OF FLUID-DYNAMICS PROBLEMS

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ABSTRACT

Computational Fluid Dynamics (CFD) tools provide users with accurate simulations. Their main drawback is the computational cost, specially when complex phenomena are modelled. For this reason, machine learning approaches have been taken, reducing computational cost while keeping good accuracy.

One application that could benefit from these approaches are predictive digital twins. When a user wants to estimate the flow behaviour under real operation conditions, sensors are used. Usually, sensors provide very accurate measurements, but as they are placed only in certain points of the domain, the obtained measurements are sparse.

We propose a Deep Learning approach to obtain a high-resolution estimation of the flow around an obstacle when only low-resolution data of the most relevant fields of the flow (pressure and velocity) is available. For this work, a database of unsteady flows around a cylinder has been generated using the OpenFoam software. Then, after a post-processing step, the database is obtained in both low-resolution and high-resolution. The analysed domain is discretized using the levelset, so the data is obtained as a grid. This structure of the data allows us to make use of Convolutional Neural Networks (CNN).

The proposed method is trained in two steps. First, an Adversarial Autoencoder (AAE) is trained to learn a low dimensional codification of the pressure and velocity fields (P, Ux, Uy) from the low-resolution data. The decoder is trained to generate the pressure and velocity fields in low and high-resolution, which means it can recover the high-resolution information of the flow taking the low-resolution measurements as input. Then, a second network is trained to predict the development of the flow. The network is a Structure Preserving Neural Network (SPNN) [1], which calculates and integrates the evolution of the flow in the low dimensional space. The SPNN ensures that the prediction is thermodynamically consistent, improving the robustness and generalization of the neural network. The thermodynamic consistence is achieved by the GENERIC (General Equation for Non-Equilibrium Reversible-Irreversible Coupling) [2] formalism. Finally, the decoder of the AAE is applied to recover the high-resolution flow fields from the low dimensional space.

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Computational methods for wind energy
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AEROELASTIC RESPONSE OF THE NREL-15 MW WIND TURBINE ROTOR USING FLUID-STRUCTURE INTERACTION MODELING

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ABSTRACT

This work aims at estimating the aeroelastic response of the blades of a standalone NREL-15 MW wind turbine [1]. To this aim, we will use a high-fidelity fluid-structure interaction solver based on a two-way coupling between a computational fluid dynamics (CFD) solver and a computational structural dynamics (CSD) solver [2], which has already been validated for lower-scale wind turbines. We will compare numerical results with those obtained from the engineering-based solver OpenFAST, developed by the National Renewable Energy Laboratory (NREL). The CFD solver adopts a Large Eddy Simulation (LES) approach, which resolves large scales and models the small subgrid scales through the Smagorinsky model. Rotor blades are modeled using the actuator line model, whereas the tower and nacelle are modeled using the immersed boundary method [3]. The CSD solver models the blades as cantilever beams using a modal approach under the assumption of linearity. A preliminary validation of the structural eigenfrequencies for the new wind turbine has been carried out, providing good agreement with the results available in the literature. The CFD-CSD results are compared with those obtained by the OpenFAST solver, which instead models the aerodynamic effect using the Blade Element Momentum (BEM) theory. This solver allows the user to employ two alternative models for the structural behavior of the blades, ElastoDyn and BeamDyn, using linear modal dynamics and geometrically exact beam theory, respectively. In the first set of simulations, a laminar, sheared wind profile defined by a power law is imposed at the inlet points of the computational domain. Results show that the tower shadowing effect evaluated by the CFD solver produces a considerable degradation in the turbine performance, while this effect is not captured by OpenFAST. A good agreement is found for the mean out-of-plane deflection along the blade, which represents the most influential deformation, despite notable differences in the in-plane deflections. The nature of these discrepancies could be attributed to the limited validity of the linear assumptions in the structural solver in the context of large-scale wind turbines and the non-negligible differences in the fluid modeling of the wake. Further details and analysis will be provided in the extended abstract.

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Advances in computational mechanics for flow-induced vibrations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICS-INFORMED NEURAL NETWORK-BASED MODELING OF THE ELASTIC RECONFIGURATION OF A PLATE UNDER FLUID FLOW

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ABSTRACT

This work focuses on the modeling with Physics-Informed Neural Networks (PINNs) of the reconfiguration of a flexible plate subjected to a perpendicular two-dimensional (2D) fluid flow. A PINN is a hybrid data-driven and physics-based model, wherein the neural network acts as a solver harnessing physical laws through additional loss functions. They are universal function approximators and meshless, by using backpropagation to compute derivatives from Partial Differential Equations (PDEs). PINNs have been applied to Vortex-Induced Vibrations (VIV) of rigid bodies, where the Fluid-Structure Interaction (FSI) remains stationary owing to the structural reference frame. However, this application does not extend to deformable multidomain interfaces. The latter are challenging for PINNs since their motion induces a relative displacement of collocation points, resulting in the simultaneous presence of all states within the training domain. Herewith, this work features a plate reconfiguring in a 2D fluid flow to showcase the representation of deformable FSI with PINNs. Indeed, plate reconfiguration is a nonlinear problem that exhibits VIV and flutter instability. Two PINN-based models are proposed for the static and dynamic reconfigurations. Both couple two PINNs to represent the structure and fluid respectively. The structural PINN integrates boundary conditions and PDEs of a fixed-free Euler-Bernoulli beam, on which only the pressure drag is applied. The fluid PINN is based on the incompressible Navier-Stokes equations with boundary conditions to represent a 2D infinite flow. The structural PINN provides forces to the fluid PINN, while the latter supplies pressure to the former. The fluid and the plate have respective sets of collocation points, where the PDEs and conditions are softly constrained. When deformation of the plate occurs, the associated points move, and the intersected fluid ones are masked with weights. The structural and fluid PINNs are trained simultaneously using a common loss that combines both formulations. Temporal terms in the PDEs and initial conditions are integrated into the framework to account for dynamic reconfiguration. A sequential training of both PINNs per time step is conducted to enforce causality. The models are verified with numerical results from a finite element model and validated with experimental data from a wind tunnel. In further work, these models will be extended to high-speed flows by applying a potential flow description and approximating the plate pressure drop. Yielding meshless and data-integration properties, PINNs offer flexible forward and inverse solvers to support conventional FSI numerical models.

Keywords: fluid-structure interaction, plate reconfiguration, Physics-Informed Neural Networks (PINN)

Contact and interface mechanics: Modeling and computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMPLEMENTING AND EXPERIMENTALLY VALIDATING PENALTY CONTACT IN COSSERAT ROD MODELS TO EFFECTIVELY MODEL CONTACT SCENARIOS IN THE FIELD SOFT MATERIAL ROBOTICS

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ABSTRACT

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Soft robotics is an aspiring field of research that aims to enhance and diversify the field of classical robotics by incorporating flexible structures and soft materials. Through their low structural stiffness and the related softness, these robots are advantageous when operating in unknown environments, interacting with objects with various topology or enabling save human-robot interaction. Despite this prominent advantage, the closely associated contact behavior of soft robots has hardly been researched to date.

In order to close this gap, the presented work aims to establish mechanical contact modeling in the field of soft robotics and make them accessible to researchers. In a previous publication the necessity to consider contact modeling has been demonstrated [1].

In a next step a contact modeling is presented for cosserat rod models. Due to their low computational cost and simplicity while still modeling the robots sufficiently these rod models are well established in the filed of soft robots and beyond. Basing the presented work on a toolbox [2], that is frequently used in the field of soft robotics, the contact model will be more accessibly and adaptable for other researchers that work in the same research area.

In this work a penalty contact is implemented in a cosserat rod model, presented in the toolbox, to model contact normal forces. These forces then act as an external force on the beam and can deform the beam due to contact. In addition, tangential forces are implemented to account for frictional contact. Both, frictional and non-frictional contact is validated by means of experiments. It is compared and presented how frictional and non-frictional contact influence and effect various contact scenarios. Therefore, multiple contact examples are presented. The work shows that contact between the robot and its environment not only does not have to be avoided. On the contrary contact can also be deliberately used to increase the stability of soft structures and thus, for example, reach a desired point or increase a load-bearing capacity.

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Immersed-boundary variational methods: Theory, data structures, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE VIRTUAL ELEMENT METHOD ON APPROXIMATE DOMAINS: A NEW STRATEGY FOR HIGHER ORDER DISCRETIZATION OF PDES WITH CURVED BOUNDARY

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ABSTRACT

The virtual element method is an extension to polytopal tessellations of the finite element method. Since its introduction in the early 2010's the method has quickly gained the attention of the scientific community, thanks to its versatility, its robustness (in particular with respect to the shape of the elements), and its potential for high accuracy (the discretization can be designed to be of arbitrarily high order). We propose its combination with a shifted boundary approach, to handle problems on domains with curved boundaries, approximated by polygonal/polyhedral domains, with emphasis on the ones obtained as the union of squared/cubic elements out of uniform structured meshes. In order to ensure efficiency we devise a novel static condensation strategy acting on the edges of the decomposition, that allows to avoid the proliferation of degrees of freedom for polygonal/polyhedral elements with a large number of small edges/faces. We show, both theoretically and numerically, that resorting, possibly only in the proximity of the boundary, to the use of the virtual element method allows to satisfy, for any order, the assumptions required for the stability of shifted boundary type methods, thus allowing to fully exploit the potential of higher order discretizations in the presence of curved boundary.

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REDUCED ORDER MODELS OF PARTICLE-LADEN FREE SURFACE FLOW

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ABSTRACT

Particle-laden free surface flow arises in many applications from spiral separators to Bostwick consistometers in the food industry. I will review lubrication theory for particle-laden flow on an incline for viscous fluids for monodisperse and bidensity flows in which the dynamics is dominated by a balance between hindered settling of particles and shear-induced migration through the layer. I will present a new model for bidisperse particle-laden flows and will discuss the behavior of the flows in multiple regimes including the case where particles preferentially settle to the substrate and where the particles stay entrained in the flow and concentrate at the leading edge of the flow. The reduced order models take the form of systems of conservation laws which exhibit singular shocks in the high volume fraction limit.

Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTATIONAL ERROR ESTIMATION FOR THE MATERIAL POINT METHOD USING ERROR TRANSPORT

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ABSTRACT

The Material Point Method (MPM) is widely used for challenging applications in engineering and animation but lags behind some other methods in terms of error analysis and computable error estimates. The complexity and non-linearity of the equations solved by the method and its reliance both on a mesh and on moving particles makes error estimation challenging. It is also the case that there is considerable variation in the order of accuracy of the different methods in the presence of grid crossing and large deformations. Furthermore, the overall time dependent nature of MPM also complicates matters as both space and time errors and their evolution must be considered thus leading to the use of explicit error transport equations. The preliminary use of an error estimator based on this transport approach has yielded promising results in the 1D case, [1] including for cases in which there is a massive amount of grid crossing leading to a loss of accuracy for conventional MPM methods.

The extension of the error estimation approach to two space higher dimensions is considered and together with additional algorithmic and theoretical results, shown to give promising results in preliminary computational experiments. The main approach adopted extends [2] to estimate the underlying error in the mappings that define the acceleration at nodes and in the mappings from nodes to particles. Some preliminary analysis is also undertaken to show how these errors at each step influences the overall error and how errors in stresses have an impact on the acceleration error and may reduce its accuracy. Finally this idea and these results are illustrated by undertaking computation experiments on standard test problems such as the vibrating ring problem used by Brannon and colleagues [3]. Finally, the difficulties faced in extending this approach to challenging real world problems are considered.

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Data-driven modeling and design of materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GRADIENT-FREE NEURAL TOPOLOGY OPTIMIZATION

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ABSTRACT

Gradient-free optimizers allow for tackling problems regardless of the objective smoothness or differentiability, but they require many more iterations to converge when compared to gradient-based algorithms. This has made them unviable for topology optimization due to the high computational cost per iteration of these problems. We propose a pre-trained neural reparameterization strategy that leads to an order of magnitude decrease in iteration count when optimizing the designs in latent space. We demonstrate this via extensive computational experiments in- and out-of-distribution with the training data. Although gradient-based topology optimization is still more efficient for differentiable problems, such as compliance optimization of structures, we believe this work will open a new path for considering problems when gradient information is not readily available (e.g. fracture).

Numerical modeling of granular and multiphase flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT OF A POLYHEDRAL DEM METHOD FOR SIMULATING THE RELOCATION OF NUCLEAR FUEL DURING A LOCA.

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ABSTRACT

During a Loss of Coolant Accident (LOCA), fuel rods are heated by the residual power. The resulting increase of internal pressure leads to a ballooning of the cladding which allows the fuel to relocate and, if there is a rupture, to disperse into the primary circuit. The exact amount of relocation and dispersal must be assessed precisely.

Here, we propose to assimilate the fragmented fuel to a granular medium and implement a Discrete Element Method (DEM) to model the behavior of fragments within the rod. The aim is to describe their relocation in the swollen areas through the analysis of key parameters, notably the packing fraction of relocated fuel along the rod.

This model echoes previous DEM-focused numerical simulation works on fragment relocation [1], [2]. Some of these models have limitations in terms of representation (2D model, spherical shape of fragments, fluid effect not considered), which we aim to overcome by creating a realistic 3D model to represent the main features of the fuel rod during a LOCA:

- The complex shape of the fragments;
- The deformation of the cladding and the interaction of fragments with the inner wall;
- The interaction of fuel fragments with fission gases and the confinement gas;

The initial developments aimed to adapt the discrete element method to arbitrary polyhedral geometries, adopting a method based on sphero-polyhedra. This method allows to facilitate the contact detection stage, which is computationally expensive and challenging to implement for complex geometries.

Verification and validation test cases of the polyhedral DEM method have been conducted. They serve as benchmarks for applied simulations aimed at studying the effect of various parameters (size and shape distribution of fragments, polydispersity, deformation of the swollen zone) on fuel relocation in the case of a dry granular medium.

Further developments are in progress to address the effects of fragment interaction with cladding walls and fission gases. Various coupling methods with DEM are being explored, and their selection is the subject of current research efforts.

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Modeling and simulation of coupled processes in geological media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ON IN-PLANE FLOW THROUGH FRACTURE PHENOMENA USING STABILIZED FINITE ELEMENT METHODS

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ABSTRACT

A reduced dimension fracture flow model (GG22) derived from the Navier-Stokes equations was recently proposed [1]. This model accounts for time-space varying apertures, transient flow, moderately high Reynolds numbers, turbulence, and satisfies conservation of energy. In comparison with the standard Poiseuille flow model, the GG22 equations capture transient and inertial phenomena. The solution of this system of nonlinear partial differential equations was previously obtained for one dimensional [2] and axisymmetric fractures [3] using the finite volume method. In this context, the present research focused on extending the solution of the GG22 equations to two dimensional fractures. The model resembles the compressible two-dimensional Navier-Stokes equations as the aperture acts as a pseudo-density in the balance of mass equation. The solution was obtained using stabilized finite element methods to avoid instabilities generated by advective terms in the balance of linear momentum equation. The verification of the solution was done against analytical solutions [1] in both one and two-dimensional examples. The model could capture re-circulation effects that were not addressed in previous research that appear due to changes in the aperture, high flow rates and discontinuities in the mesh.

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Structure-preserving discretization of multiphysics systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GENERIC-BASED MIXED FINITE ELEMENTS FOR COUPLED THERMOMECHANICAL PROBLEMS

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ABSTRACT

The GENERIC formalism provides a versatile framework for the formulation and structure-preserving discretization of coupled multiphysics problems. GENERIC (General Equation for Non-Equilibrium Reversible-Irreversible Coupling) relies on an additive decomposition of the evolution equations into reversible and irreversible processes. After the selection of appropriate state variables, GENERIC is formulated as state space model of the coupled problem under consideration. Correspondingly, related numerical methods for coupled thermomechanical problems typically rely on an approximation of the state variables at hand. Using the finite element method for the discretization in space, the GENERIC-based formulation can be viewed as generalization of displacement-based finite elements for isothermal mechanical problems. To improve the numerical approximation capabilities of displacement-based finite elements a plethora of mixed finite element formulations has been developed over the last decades. The goal of the present work is to extend the GENERIC framework to accommodate mixed finite elements for the structure-preserving discretization in space and time. The GENERIC-based application of mixed finite elements is illustrated with the problem of large strain electro-thermo-elastodynamics.

Computational design of mechanical metamaterials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A REDUCED ORDER MODELING BASED FETI-DP SOLVER FOR MECHANICAL METAMATERIALS

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ABSTRACT

The recent advances in additive manufacturing technologies are pushing the development of architected cellular materials, such as the so-called mechanical metamaterials, to a new stage. These multiscale heterogeneous lattice structures can be tailored at the level of the unit-cell to achieve exceptional mechanical properties that are difficult to find in conventional materials. However, because of the possibly huge number of cells, the evaluation of their mechanical response is challenging due to high computational cost and memory requirements. In this work, we develop a fast and accurate solver for the full fine-scale analysis of gyroid-like mechanical metamaterials. Our strategy is based on unfitted domain methods, which avoid computationally costly meshing routines. Upon this choice, our main purpose is to exploit the natural domain decomposition of the macro-structure into unit-cells by designing an efficient FETI-DP solver. Importantly, we apply localized projection-based reduced order models for the approximation of the main substructuring operators. Ultimately, this results in an accurate and scalable algorithm which avoids a significant number of local factorizations and considerably reduces the online computational cost. The applicability of our methodology is shown on a variety of 2D and 3D examples, for different geometries and load terms: the developed solver shows excellent accuracy on large enough test problems, with good gains in running time with respect to a high-fidelity solver.

Geomechanics of the cryosphere
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A COUPLED FLOW-FLEXURE-FRACTURE MODEL FOR SHALLOW ICE SHELVES

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ABSTRACT

Glacier ice deforms via a combination of viscous flow and viscoelastic flexure. However, due to the computational complexity of modeling viscoelastic materials, global ice sheet models currently treat glacier ice as purely viscous. This pragmatic approach renders ice sheet models unable to describe large-scale phenomena emerging through the viscoelastic properties of ice, such as the chain-reaction lake drainage events which have been proposed to help disintegrate enormous swaths of Antarctic ice shelves. This project builds on MacAyeal et al. (2021, Journal of Glaciology) to develop a process-scale ice shelf model coupling viscous flow with viscoelastic flexure, while using approximations which are computationally cheap enough to eventually incorporate into global ice sheet models. We solve the two-dimensional Shallow Shelf Approximation (SSA) for viscous ice shelf flow alongside a thin-plate approximation for viscoelastic flexure. Additionally, we apply a continuum damage description to approximate the effect of fracture on rheology. Since most global models already solve the SSA to describe the viscous flow of ice shelves, our coupled flow-flexure model will be easily adaptable into ice sheet models. Ultimately, our work will help elucidate large-scale ice shelf behaviour which emerges through the viscoelastic properties of ice.

Uncertainty quantification in structural dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

UNCERTAINTY QUANTIFICATION OF LARGE STOCHASTIC NONLINEAR DYNAMICAL SYSTEMS USING A NOVEL NON-INTRUSIVE ROM

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ABSTRACT

Uncertainty quantification (UQ) or reliability analysis of large nonlinear stochastic dynamical systems demands huge computational costs. Often, these systems are solved using commercial software or a black-box solver, where access to the source code is restricted. In this situation, UQ of such systems becomes computationally challenging. The cost has two components: (i) cost due to large physical dimension, and (ii) cost due to large stochastic dimension. While the first issue is addressed using a non-intrusive reduced order model (ROM), the latter is still a challenging problem within the framework of a non-intrusive ROM. While the literature on non-intrusive ROMs [1] is growing, their applicability in large stochastic dimension is still an unaddressed issue. This work is aimed at addressing this issue.

The key challenge lies in building a high-dimensional interpolation or approximation scheme between random variables or process to reduced space solutions. In our recent previous work [2], we have addressed this challenge for a linear problem with random process excitation. The interpolation was carried out using feed-forward neural network in tandem with principal component analysis. In the proposed work this methodology is extended to nonlinear systems. Here we have developed a proper orthogonal decomposition-based ROM that uses a long short-term memory (LSTM) network for the interpolation. An LSTM has a memory cell that remembers important information from the past, which is crucial in the analysis of nonlinear dynamical systems. The accuracy of the developed ROM is numerically validated on a beam on a nonlinear Winkler foundation model subjected to both stationary and non-stationary random excitations. The nonlinearity in the foundation is modeled using Mostaghel's spring, which shows bilinear hysteresis behavior. The ROM is later used in estimating the failure probability for different thresholds. The numerical results show that the proposed ROM is accurate and efficient in estimating the failure probabilities. The ROM gains a speed-up of about 300 in the online stage.

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RESIDUAL DIFFUSION MODELING FOR KM-SCALE ATMOSPHERIC DOWNSCALING

Tarini Bhatnagar[1], Morteza Mardani[1], Noah Brenowitz[1], Yair Cohen[1], Jaideep Pathak[1], Chieh-Yu Chen[1], Cheng-Chin Liu[2], Arash Vahdat[1], Karthik Kashinath[1], Jan Kautz[1] and Mike Pritchard[1]*

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ABSTRACT

Global Climate Models are instrumental in informing and providing insights into climate systems over larger time scales, although at a coarse resolution. Many applications of weather and climate data such as risk assessment, regional climate change studies require higher resolution, km-scale forecasts. Machine Learning for dynamic downscaling for regional simulation is attractive, but computationally expensive. Statistical downscaling, an inexpensive alternative, lacks the fidelity of dynamic downscaling. Here, we present a cost effective, generative diffusion model, Corrector Diffusion (CorrDiff) for downscaling coarser resolution (25km) global weather data to a higher resolution (2km) over a subset of the globe. With basic GPU hardware and with an unoptimized code, CorrDiff inference is about 38x faster, and 1800 x more energy efficient than running Weather Research and Forecasting (WRF) on CPU. With the current focus on generation quality, and not on optimizing inference speed, more gains on GPU could be easily anticipated.

Computational mechanics for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CRYSTAL PLASTICITY FINITE ELEMENT CREEP MODELING OF POWDER BED FUSED 316H STEEL

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ABSTRACT

316H Stainless steel is a popular material for high-temperature applications. However, accurately predicting the long-term performance of additively manufactured components in service environments remains challenging due to a lack of understanding of very long-term microstructural stability under load. In this study, we investigate the anisotropic creep deformation behavior of an additively manufactured 316H polycrystal, produced using the laser powder bed fusion method. To do so, we generate a high-fidelity finite element mesh, using data received Manufacturing Demonstration Facility at Oak Ridge National Laboratory, that accurately represents the microstructure of the material. Creep is modeled using a MOOSE-based crystal plasticity finite element framework, DEER, to study the role of grain structure and orientations in the creep response of the AM microstructure. In this work, we study the effect of grain morphology, the aspect ratio of grains, strategies to incorporate the complex orientation distribution within the microstructure into the FE mesh of the polycrystal, and the effect it has on creep performance. Through this investigation, we aim to improve our understanding of the structure-property relationship in additively manufactured in 316H stainless steel, thus helping us predict and optimize its long-term performance.

SciML in the real world
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN CONSTITUTIVE RELATIONS: MULTISCALE MODELING AND EXPERIMENTAL INFERENCE

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ABSTRACT

The talk addresses the challenge of computing complex phenomena at the scale of applications. In addition to the universal laws (balance of mass, momenta etc.), these phenomena require a constitutive (closure) relation that describes the behavior of the medium at the scale of applications. Such behavior can be nonlinear, nonlocal, anisotropic, history dependent etc., and thus impossible to characterize to the desired level by the classical approach of postulating a parametrized relation and fitting the parameters to selected experiments. The talk describes two broad approaches to using data-driven methods to overcome this challenge. The first approach is multiscale modeling where one recognizes that the effective behavior at the scale of applications is determined by physics at multiple length and time scales: electronic, atomistic, domains, defects etc. The data-driven constitutive relation is obtained as a neural approximation is trained using data generated by repeated solution of the small scale problem. The second approach seeks to infer it from automated experiments that are not amenable to easy inversion. The talk will describe these approaches, challenges they raise and strategies to overcome them. The ideas will be illustrated with applications from materials science and geology.

ASSESSMENT OF FULLY EULERIAN PHASE-FIELD FRAMEWORK FOR SHIP HYDRODYNAMICS WITH ICE INTERACTION

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ABSTRACT

With ice cover in the Arctic region shrinking over time, the region has garnered strategic interests for shipping activities. The development of robust ice-going ships, that can navigate ice fields with minimal resistance and extreme load on the hull, is an emerging application of multiphase fluid-structure interaction. The complex and coupled nonlinear dynamics associated with ship-ice contact on a free surface is challenging to predict and analyze sufficiently via theoretical and experimental methods. High-fidelity numerical models for ship-ice interaction on a free surface, and the resulting force analysis, are therefore imperative for the optimization of ice-going ship hull design for Arctic region operations.

Ship-ice interaction is a complex system involving interaction between floating structures and surrounding free surface, and contact between solids. These interactions happen amid large translational and rotational motions of the floating structures. When using an arbitrary Lagrangian-Eulerian (ALE) framework [1] to model the contact dynamics of structures on a free surface, maintaining the mesh quality in the region between the approaching structures poses a major challenge. A multiphase fully-Eulerian framework is therefore advantageous for this application, as it is able to model the continua of all fluids and solids involved in a Eulerian frame. A novel multiphase fully-Eulerian framework employing a phase field formulation to describe the interfaces between the phases has been developed [2]. Rigorous validation and a complete force analysis flow are now required to apply it to study ship-ice interaction.

Accurately modeling how an afloat solid interacts with surrounding free surface flow is a premise for studying the contact between structures on a free surface. We consider the hydrodynamics arising from flow across a Wigley hull as a relevant benchmark problem and solve the problem with the fully Eulerian framework. We study the wave run-up profile on the hull and build a workflow to analyze the resulting resistance and extreme load on the hull. We finally present a simple ship-ice interaction on a free surface simulated with the solver to investigate the contact force between solids.

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Continuum biomechanics of active systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MATERIAL CHARACTERIZATION AND PARAMETER IDENTIFICATION OF PERIODONTAL LIGAMENT CONSIDERING TENSION-COMPRESSION ASYMMETRIC MODULI AND NONLINEAR BEHAVIOR

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ABSTRACT

Background and purpose: Periodontal ligament (PDL) is a complex biological soft tissue that connects teeth and alveolar bone. The hydrostatic stress in the PDL are generally considered as a key factor to trigger orthodontic tooth movement. Accurate characterization of the material properties of the PDL holds the potential to influence the stress in the PDL during orthodontic simulations using finite element analysis, therefore to impact the clinical orthodontic treatment plan. Studies on the material properties of the PDL has been ongoing for decades. However, previous research has not adequately taken into account the distinct properties of the PDL under tension and compression. PDL is softer under compression than tension, and has greater compressibility under compression, which significantly affects the hydrostatic stress within it. The proposed work considers the different elastic modulus and Poisson's ratio of the PDL under tension and compression, and further introduces nonlinearity to the tension stage.

Methods: Using the commercial finite element solver Abaqus, a customized constitutive model UMAT, and the simulation automation software Isight, the nonlinear tension-compression asymmetric constitutive model is achieved. By utilizing in-vivo experimental data, the material properties of the PDL are characterized. Based on the constitutive model, an orthodontic process is simulated and the hydrostatic stress in the PDL is evaluated.

Results and conclusions: The results show that considering the nonlinear and asymmetric mechanical behavior of PDL in tension and compression can significantly reduce the evaluated compressive stress in the PDL, which is more realistic and closer to the orthodontic theory.

The phase field method for fracture: Theory, numerics, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A VARIATIONALLY-CONSISTENT PHASE-FIELD COHESIVE ZONE MODEL FOR MIXED-MODE FRACTURE BASED ON ENERGY DECOMPOSITION SCHEME

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ABSTRACT

In rocklike materials, mode I and II fracture toughness are distinctive while the compressive strength is much greater than the tensile strength. Besides, mixed-mode fractures instead of pure mode I or II fractures occur under complicated load cases in those materials. Therefore, to capture the mixed-mode cracking process, we developed a mixed-mode phase-field cohesive zone model based on the unified phase-field theory proposed by Wu. The model was built based on a strain energy decomposition scheme, and for each mode, there is an independent degradation function. Thus, independent values of strength and toughness can be given for different failure modes. A simple mixture rule of fracture toughness was introduced to describe the transition between different failure modes. The model can keep variational consistency perfectly and governing equations for displacement- and phase-field, which was never reported in other works. Several numerical examples verified the effectiveness and flexibility of this work. The present work showed a simple but effective way to simulate mixed-mode fracture.

Computational methods for wind energy
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CHARACTERIZING THE EFFECTS OF INFLOW TURBULENCE ON THE UNSTEADY LOADS AND WAKES OF WIND TURBINES

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ABSTRACT

Wind turbines operating under extreme wind conditions are subjected to high wind speeds and turbulent intensities. In this scenario, the turbine blades experience high degree of unsteady loading due to flow separation. If the frequency of the vortex shedding due to the massively separated flow from the blades coincides with the blade's natural frequency, stall or vortex induced vibrations occur which can lead to fatigue or failure of the turbine blades. In this study, the effects of varying the inflow wind speed and turbulent intensity on the unsteady loads and wake characteristics are investigated for the rigid NREL Phase VI turbine under axial-flow conditions. Blade-resolved simulations are performed using the Improved Delayed Detached Eddy Simulation (IDDES) hybrid RANS-LES turbulence model. We consider two methods to generate the inflow turbulence. In the first approach, turbulent conditions are specified at the inlet, and the decay of turbulent kinetic energy is estimated from the inlet to the turbine. The second method injects resolved turbulence using a synthetic turbulence generator. A preliminary investigation was performed for wind speed of 20m/s and inflow turbulent intensity of 0.5%. The IDDES turbulence model accurately predicted both the mean and unsteady loads, and the flow separation. To further validate the performance of the model, the power spectral density (PSD) based on the thrust coefficient was compared with the experimental data [1] at five spanwise locations on the blades. The model correctly captured the primary shedding frequencies at all locations. Additionally, the slope of PSD curve in the high frequency range shows good agreement with -5/3 slope. In addition to predicting the unsteady loads and performing comparison studies of power spectral density, the effects on velocity deficit and turbulent intensity are also examined both in the near- and far-field wake regions.

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Advances in neural operators for scientific modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ACCURATE SOLUTION OF LINEAR OPERATOR APPROXIMATIONS USING GREEN'S FUNCTIONS BY A MULTI-LEVEL NEURAL NETWORK APPROACH

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ABSTRACT

The solution of boundary-value problems using deep learning approaches, such as the physics-informed neural networks [1] or the deep operator networks [2], have been extensively investigated in recent years. However, achieving high accuracy in the approximations obtained from these methods often remains a significant challenge. A multi-level neural network approach was proposed in [3] that allows one to iteratively reduce the errors, sometimes within machine precision, when approximating a solution using PINNs. In this work, we extend the multi-level approach to approximate linear operators using the Green operator networks (GreenONets) as described in [4]. Starting with an initial approximation of the operator, we correct the solution by considering a different Green operator network involving higher frequencies. The method enables one to iteratively reduce the high-frequency contributions present in the residuals. Numerical examples will be presented to demonstrate the efficiency of the proposed multi-level approach.

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Multiscale, multifield, and continuum-discontinuum analysis in geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CAN MULTISCALE MICROMECHANICAL MODELS EXPLAIN THE EXPERIMENTALLY OBSERVED VARIATION IN MECHANICAL PROPERTIES OF CLEAR WOOD?

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ABSTRACT

The forests in Europe are changing in response to climate shifts and thus the ratio of hardwood in mixed forests will increase. Hardwood properties, an understudied area in the past, are now gaining prominence in research. Our investigation of the mechanical properties of South Swedish wood encompasses the softwoods species spruce as a reference and the hardwood species beech and birch. Experiments on stiffness and strength perpendicular to the grain and rolling shear exhibited considerable variation [1]. Wood, whether softwood or hardwood, is a hierarchically organized geomaterial, where the macroscopic, anisotropic mechanical properties are governed by the microstructure. The presented application of multiscale models aims to explore the influence of microstructural characteristics for an explanation of the observed macroscopic variations. A validated multiscale micromechanical model for the stiffness of softwood was presented by Bader et al. [2] and further extended to hardwood by de Borst and Bader [3]. In the latter study, the model was validated for beech and nine other hardwood species.

The experiments were conducted on prismatic clear wood specimens (50 mm width, 20 mm thickness, and 60 mm height), enabling material-level testing. However, due to thickness and annual ring distribution of the raw material, the inclination of the annual rings of early- and latewood, defining the radial and tangential direction (RT-plane) of the idealized orthotropic material, varies in the test series. The influence of this RT-plane rotation and the variation in microstructural parameters, like microfibril angle, lumen, vessel, and ray cell properties, on the global stiffness, are modelled based on multiscale models for the three investigated species. The micromechanical models are applied to obtain mean values of the nine independent components of the stiffness tensor with corresponding realistic modelling variations. These tensors are then rotated within the RT-plane to investigate the influence on the global clear wood behavior. The modelled global stiffness values are subsequently compared with the experimental results.

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Advances and applications of polytopal methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DYNAMIC CRACK PROPAGATION DUE TO THERMAL LOADS MODELED USING SCALED BOUNDARY POLYGON ELEMENTS

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ABSTRACT

Thermal shock leads to thermally-induced stresses that can trigger rapid crack propagation in brittle materials. Predicting and preventing failure due to thermal shock is therefore required in the context of designing pressure tanks or reactors for thermal power plants or in aerospace engineering. The numerical modeling of thermally-induced dynamic crack propagation is challenging for several reasons. Thermal shock problems are characterized by extreme variations of the coupled thermal and mechanical quantities with respect to space and time. In a brittle material, stress singularities occur near crack tips that need to be resolved using a suitable numerical method. Crack propagation is associated with geometry evolution, which must be captured using efficient re-meshing approaches in discrete crack modeling scenarios.

In this contribution, the above challenges are addressed using the scaled boundary finite element method (SBFEM). Being a semi-analytical technique, it excels at representing stress singularities efficiently and accurately. Stress intensity factors are obtained semi-analytically directly in the solution process. They can be evaluated on relatively coarse meshes and without the need for costly post-processing techniques. Moreover, the scaled boundary finite element method can be used on polygon meshes that facilitate local re-meshing as cracks propagate. Applications to steady-state thermally-induced crack propagation modeling can be found in [1], for example.

The fully coupled transient thermoelastic problem is solved using scaled boundary shape functions, where the displacement approximations are enriched with semi-analytical solutions of the linear-elastic thermal stress problem [2]. In the context of crack propagation modeling, mesh mapping is required when the geometry changes. This is not trivial for the auxiliary degrees of freedom associated with the supplementary scaled boundary shape functions mentioned above. We, therefore, propose an extrapolation-based mesh mapping scheme, which is suitable for thermally-induced dynamic crack propagation modeling using SBFEM. The proper choice of crack propagation increment and time step and their interplay with the crack velocity are also discussed. The proposed procedure is verified and illustrated using various numerical examples.

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Innovations in machine learning-enhanced uncertainty quantification for computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

METHODS FOR GENERATING INTERPRETABLE YIELD SURFACE MODELS WITH UQ BASED ON DATA WITH MULTIPLE SOURCES OF UNCERTAINTY

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ABSTRACT

When using machine learning (ML) methods in engineering, interpretability and robustness to noise are essential as it enhances model trust. Here, we use genetic programming based symbolic regression (GPSR), which generates free-form equations from provided mathematical operators and data. Previously, we demonstrated how using Bayesian methods such as sequential Monte Carlo (SMC) within the GPSR framework allows the generation of yield surface models with uncertainty quantification (UQ). We now look to extend SMC-GPSR to differentiate intrinsic (e.g., material scale variability) and extrinsic (e.g., measurement imprecision) sources, further enhancing model interpretability.

Our implementation for differentiating potentially confounding sources of uncertainties relies on a priori analysis of the material microstructure to identify intrinsic uncertainty terms and uniquely inform corresponding prior distributions for associated parameters within the evolving GPSR models. This is accomplished by using a thermodynamic-based analysis [1] to produce a composite function within which each sub-function connects to a microstructural characteristic of the material. The prior distributions inform the intrinsic uncertainty, while uncertainty from extrinsic sources is defined using an uninformed prior. This implementation is tested by generating training data from a known yield surface model for porous metals, the Gurson-Tvergaard-Needleman (GTN) model. Noise is artificially added to the parameters as well as the output data to simulate sources of intrinsic and extrinsic uncertainty, respectively. Assessment of the algorithm performance is determined by the successful determination of the known uncertainties in this verification test.

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16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Advances in discretization techniques, element technology, mesh adaptivity, and solution strategies for inelasticity, localization, and failure

July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A QUASI-MESHFREE METHOD FOR NONLINEAR SOLID MECHANICS ON GEOMETRICALLY COMPLEX DOMAINS USING BOUNDARY-AWARE REPRODUCING BASIS FUNCTIONS AND A PROJECTED-GRADIENT QUADRATURE SCHEME

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ABSTRACT

In many applications, domains of interest are geometrically complex containing numerous small features. These features are typically removed in a manual process to facilitate a conventional element-based meshing process. This manual defeaturing process is dependent upon the goals of the simulation and typically involves subjective heuristics. To provide a flexible and easily adaptable discretization process that is independent of the domain discretization, an element-free method is proposed in which a fine-scale triangulation of the domain is used to first discretize the fully featured geometry but then a coarse-scale element-free discretization is used to approximate the solution of the governing equations. The fine-scale triangulation can be of poor quality and extremely refined since it is not used directly to approximate the solution. The coarse-scale element-free basis can be adapted through refinement or coarsening without the need to alter the fine-scale triangulation or other geometric considerations. The element-free basis functions are constructed using a traditional moving-least-squares procedure, but the initial weighting functions are constructed using manifold geodesics for general applicability to non-convex domains.

The weak form of the governing equations is integrated using a secondary coarse-scale element-free basis and a gradient projection technique. The projected-gradient methodology ensures the necessary consistency properties to pass the patch test. The dimension of the secondary basis is chosen to be of sufficient size to ensure stability of the overall method. The overall method is termed quasi-meshfree since both meshfree and mesh-based concepts are used. Several 2D verification problems and nonlinear application examples are presented to demonstrate the overall method.

Fracture, damage and failure mechanics of cementitious materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ON THE USE OF FINITE ELEMENTS WITH A HIGH ASPECT RATIO AND COUPLING FINITE ELEMENTS FOR MODELING THE FAILURE PROCESS IN SFRC WITH DISCRETE TREATMENT OF FIBERS

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ABSTRACT

This paper describes a multiscale approach for modeling the failure processes of steel fiber reinforced cementitious materials with discrete treatment of fibers. The material is described as a composite made up by three phases: the cementitious matrix, discrete discontinuous fibers, and fiber-matrix interface. Special finite elements (named coupling elements) [1] were developed to couple independent meshes of the matrix (2D or 3D solid elements) and a cloud of steel fibers (modeled with truss elements). The complex nonlinear behavior of the interaction between concrete and fibers is modeled through a damage constitutive model and a non-rigid coupling procedure. Regular reinforcement bars can also be modeled with this technique. Initially, numerical examples with a single fiber are presented to validate the technique and to investigate the influence of its geometrical properties and its position related to crack surface. Then, more complex examples involving a cloud of steel fibers are considered. In these cases, special attention is given to analysis of the influence of the fiber distribution on the composite behavior related to the cracking process. With this proposed coupling technique any existing method to model cracks in the concrete matrix can be used without changes. In this paper the formation and propagation of cracks are modeled using solid finite elements with high aspect ratio [2,3] and a tension damage model to represent the behavior of interfaces associated to potential crack surfaces. Those interface elements are inserted in between all regular (bulk) solid elements of the concrete mesh, so that multiple cracks can also be considered.

FLEXIBLE INFINITE ELEMENTS FOR DIGITAL TWIN DEVELOPMENT OF UNBOUNDED VIBRO-ACOUSTIC MODELS

Davide Bizzarri[*12], Onur Atak[1], Hadrien Beriot[1] and Sjoerd van Ophem[23]*

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ABSTRACT

In the evolving landscape of digital modelling, there is a growing interest on incorporating 3D simulations into Digital Twin scenarios [1]. A Digital Twin is characterized by the continuous exchange of data with its physical counterpart. This introduces the need of a compact representation of high-fidelity time-domain models. Therefore, the development of numerical schemes that are compatible with model order reduction (MOR) is of paramount importance.

In the realm of unbounded vibro-acoustics, the pursuit of these compact representations becomes pivotal, enabling the Digital Twin creation for an array of objects, such as loudspeakers, gearboxes and electric motors. Combining the Finite Element Method (FEM) with infinite elements is a common way to simulate unbounded vibro-acoustic phenomena. The Astley-Leis formulation, in particular, produces frequency-independent system matrices, which are readily applicable for transient simulations. Such formulation has been successfully used, in combination with Krylov-based MOR techniques, to produce accurate and time-stable reduced order models [2].

However, in the time domain, the Astley-Leis infinite elements must be attached to (semi-) spherical FEM volumes. This lack of geometrical flexibility severely limits the efficiency of the method, especially in the case of elongated radiating/scattering objects. This study presents the flexible infinite element [3], which can be connected to arbitrarily shaped convex domain FE boundaries for transient simulations, without sacrificing accuracy.

A workflow for the automatic generation of the FEM domain around sources of interest and the runtime extrusion of the infinite elements is presented. From a software implementation perspective, the proposed element can be considered as a specialized FEM element and can be seamlessly integrated into a high-order FEM code.

The computational benefits of using the flexible formulation are highlighted. Additionally, we demonstrate how integrating the proposed method with existing MOR strategies enables cost-effective and precise transient simulations. This combination paves the way for new Digital Twin applications in the field of unbounded vibro-acoustics.

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Emerging topology and shape optimization techniques in computational design of materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE STRUCTURAL OPTIMIZATION WITH STRAIN GRADIENT EFFECTS USING SECOND-ORDER HOMOGENIZATION

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ABSTRACT

Topology optimization and multiscale structural optimization have traditionally relied on numerical homogenization techniques to describe an evolving material domain. These homogenization techniques estimate the effective properties of a composite material through analysis of a microscale domain subjected to loading defined by the macroscale's mechanical state. The transition from the macroscale (observable) space to the microscale (material) space often requires restrictions on the size, form, and deformation modes of the microarchitecture. The most widely used form of homogenization in structural design defines these restrictions in terms of the (first-order) macroscale strains, assuming a strict separation of the macro- and microscales. In contrast, second-order homogenization introduces the macroscale strain-gradient in the formulation of microscale boundary conditions to relax the scale separation conditions. With their slightly relaxed model of scale separation, second-order techniques aim to model structures with observable hierarchy, modeling structures composed of many spatially varying substructures at a manufacturable scale.

The second-order formulation introduces several challenges for design optimization that will be the focus of this work. The strain gradient introduces higher order stresses in the macroscale which require special treatment. In this work, we implement a mixed finite element scheme to enforce C1 continuity in the macroscale. In the microscale, where deformation is a function of the macroscale strain and strain gradient, more considerations are required for the application of periodic boundary conditions with ersatz materials. We present the numerical implementation of the second-order homogenization model in the context of structural optimization. Through comparison with first-order methods, the ability to model hierarchical structures is evaluated. We show the behavior of second-order stress-strain relationships with the effective density of microstructural designs, producing the effective higher order properties of an evolving second-order material. Using this model, design optimization is performed using the second-order homogenization model.

OPEN-SOURCE HIGH-ORDER RESOLVED CFD-DEM FOR NON-SPHERICAL PARTICLE-LADEN FLOW

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ABSTRACT

Particulate flows play an important role in the chemical industry. They are used in reactors (e.g., fluidized beds, spouted beds), in the transport of material (e.g., slurry transport and pneumatic conveying), separation operation (e.g., cyclone separators), and atomization operation (e.g., spray drying) to name a few. The sharp interface immersed boundary method (SIBM) is a powerful tool to simulate the flow around moving objects. Recently, our group has developed a SIBM which has many desirable properties for the direct numerical simulation of particle-laden flow: it uses a fully implicit coupling scheme, it is compatible with high-order schemes in both space and time, and it is compatible with a resolved CFD-DEM formulation, enabling the capture of particle-particle and particle-wall contacts. To achieve this, it uses a streamline upwind Petrov–Galerkin and pressure-stabilizing Petrov–Galerkin (SUPG/PSPG) stabilized formulation of the Navier-Stokes equations.

In this talk, we briefly introduce this high-order resolved CFD-DEM scheme which is implemented within the open-source CFD software Lethe [1]. We verify the high order of convergence of the scheme, and validate it using benchmark cases. The first validation case is the sedimentation of a lone particle with a Reynolds number smaller than 32. The second validation case is the rise of a positively buoyant particle at a high Reynolds number (2500). The third validation case demonstrates the stability of the scheme when particles are in contact and exhibit the classical drafting, kissing, and tumbling (DKT) behavior. Using this case, we discuss challenges related to the capture of the lubrication forces. Then, we present the extension of this scheme to non-spherical, but convex, particles. We validate the capabilities of the scheme on a benchmark sedimentation test case and discuss current challenges and future directions for this highly efficient computational model.

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DATA-DRIVEN COMPACT PHOTOCURRENT MODELS

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ABSTRACT

Understanding radiation response of microelectronic circuits is facilitated by high-level circuit simulations of radiation effects, which require computationally efficient compact radiation models. Currently, development of such models is dominated by analytic approaches, which invoke physical assumptions to render the governing equations solvable in closed form. Violation of these assumptions can reduce the accuracy of the models and/or limit their scope.

This talk will focus on alternative, data-driven approaches for the development of compact radiation models. We will first review recent efforts to develop such models using projection-based model order reduction (POD-based ROM), dynamic mode decomposition (DMD) and operator inference (OpInf). All these models are discrete or continuous time dynamical systems simulating the internal state of the device and so, their learning requires snapshots of this state and for the ROM model – access to the discretized governing equations. Dependence of the model development process on the availability of this information presents some problems because the internal state of a device cannot be measured in a laboratory setting and the discretized equations may be too complex or unavailable for commercial codes.

Gray-box models (GBM) informed by device physics provide an effective way to resolve many of these issues. GBMs can be viewed as a non-intrusive ROM that does not require access to the discretized governing equations and/or snapshots of the internal device state. GBMs are particularly attractive when (i) the main simulation goal is a quantity of interest (QoI) such as device response to radiation, rather than the internal state of the device itself, and (ii) the dynamics of this QoI can be represented by a small number of latent states.

In this talk we demonstrate the appropriateness of the gray-box approach for the development of compact radiation models by formulating and testing a GBM for the delayed photocurrents in a PN-junction diode. The GBM is based on a state-space system representation in which the structure of the state equation is informed by the nonlinear Ambipolar Diffusion Equation. We also compare this GBM with a purely black-box neural ODE model, which does not assume any prior physics knowledge and attempts to learn the dynamics of the device response solely from data. In so doing we aim to assess how well such black-box models can perform under the model and data size constraints inherent to compact radiation modeling.

16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics

July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPLICIT SYNCHRONOUS PARTITIONED SCHEME FOR COUPLED REDUCED ORDER MODELS BASED ON COMPOSITE REDUCED BASES

Amy De Castro[1], Pavel Bochev[2], Paul Kuberry[2] and Irina Tezaur[2]*

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ABSTRACT

In this talk we will present a method for the partitioned solution of coupled interface problems involving combinations of projection-based reduced order models (ROM) and/or full order methods (FOMs). The method builds on a reconstruction-based partitioned scheme, which starts from a well-posed formulation of the coupled interface problem and uses its dual Schur complement to obtain an approximation of the interface flux. Explicit time integration of this problem decouples its subdomain equations and enables their independent solution on each subdomain.

Extension of this partitioned scheme to coupled ROM-ROM or ROM-FOM problems requires formulations with non-singular Schur complements. To obtain these problems, we project a well-posed coupled FOM-FOM problem onto a composite reduced basis comprising separate sets of basis vectors for the interface and interior variables, and use the interface reduced basis as a Lagrange multiplier.

Our analysis confirms that the resulting coupled ROM-ROM and ROM-FOM problems have provably non-singular Schur complements, independent of the mesh size and the reduced basis size. In the ROM-FOM case, analysis shows that one can also use the interface FOM space as a Lagrange multiplier. We will illustrate the theoretical and computational properties of the partitioned scheme through reproductive and predictive tests for a model advection-diffusion transmission problem.

Acknowledgments

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Advances in multi-scale, multi-material, and multi-component Topology Optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A HYBRID STRUCTURAL OPTIMIZATION APPROACH FOR MULTISCALE DESIGN OF ARCHITECTED COMPOSITES

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ABSTRACT

Fiber reinforced composites (FRCs) are the most widely used multiscale materials owing to their excellent mechanical properties. Despite their simple microstructure, FRCs can accommodate a wide range of property variations. However, they are typically restricted to simple designs due to limitations of the conventional manufacturing processes. Advanced manufacturing methods such as material extrusion additive manufacturing can realize FRCs with complex microstructural variations (e.g., via controlled orientation and deposition of fiber-filled polymers) akin to those found in natural composites like wood and bone. This paves the way for optimal multiscale design of composites specifically tailored to prescribed performance requirements through simultaneous optimization of macroscale topology and the microscale fibrous microstructure, thus leading to architected composites. Architected composites can unlock the full potential of FRCs and lead to lighter, stiffer, stronger, and more durable structures with applications in sectors such as aerospace, automotive, and infrastructure.

Homogenization-based structural optimization methods for multiscale design of architected composites have been popular due to their computational efficiency. These methods typically optimize the distribution of microstructure orientation in conjunction with the macroscale topology and necessitate a dehomogenization step to realize a manufacturable two-scale design. However, the dehomogenization step typically introduces a discrepancy between the optimal and dehomogenized designs due to unavoidable singularities in the orientation field. To overcome this problem, we developed a hybrid optimization approach that combines nested and simultaneous analysis and design formulations (NAND and SAND). Specifically, we employ the SIMP formulation to parametrize the macroscale topology while using the level sets of a distance field for the local fiber orientations. Following the traditional topology optimization approach, the design-dependent response of the structure is obtained from solving the elasticity equations sequentially in a nested fashion. However, the fiber orientation encoding distance field is obtained implicitly by concurrently minimizing the residual of the Eikonal equation alongside the desired optimization objective, thus forming the simultaneous aspect. This hybrid approach ensures that the optimal and realized designs have no discrepancies, retains the design freedom (which is otherwise restricted in level set based formulations), and ensures that a feasible design is available provided the Eikonal equation residual is fully minimized. We demonstrate the efficacy of this approach in 2D and 2.5D (i.e., laminates) with optimal stiffness requirement driving the designs.

Constitutive modeling of complex materials with machine learning and artificial intelligence
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ACCOUNTING FOR ELASTO-PLASTICITY IN CONSTITUTIVE ARTIFICIAL NEURAL NETWORKS

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ABSTRACT

In today's industry, we are facing constantly advancing manufacturing processes that result in new materials with improved characteristics such that the material behavior can be better and better exploited. However, the question arises on how to accurately predict the mechanical behavior of these new materials. Thus, new material models are required. But with increasing complexity of the material, the formulation of a material model is equally becoming more complex. New material models are often designed as a combination of new models and a combination of already existing, sophisticated formulations. With this, we may ask which model fits best to the material behavior that should be modeled. To facilitate the choice, we make use of machine learning to predict the mechanical behavior through constitutive artificial neural networks (CANNs). This approach has been successfully applied for elastic material behavior for example by Linka et al. [1]. The extension to inelasticity has recently been published by Holthusen et al. [2].

However, elasto-plastic behavior has not yet been captured but is one major inelastic effect. The lack of this extension leads to a novel formulation presented in this work. We propose a constitutive artificial network based on the works given above that captures not only elastic but also plastic material behavior. For this, we combine two separate feed-forward networks for the Helmholtz free energy and a potential from which we define the yield function in a recurrent neural network. The model’s performance is demonstrated on training and testing on artificial data in a first step. With this, the efficiency of the novel formulation is presented.

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Immersed-boundary variational methods: Theory, data structures, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ON THE STABILITY OF A FICTITIOUS DOMAIN APPROACH FOR FLUID STRUCTURE INTERACTION PROBLEMS

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ABSTRACT

We review the stability properties of our fictitious domain approach for fluid structure interaction problems.
Some properties are already well known, including the unconditional stability in time and the well posedness of the discrete system for several choices of finite element spaces.
In this presentation we focus on the coupling terms that, as known, require a careful computation of the intersection of the meshes related to the fluid and the solid. We will show that, as expected, the presence of small intersections does not cause problems on the quality of the approximation.

Towards predictive digital twins: Innovative algorithms for physics-, data-assisted and hybrid modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NEW APPROACH TO COMBINE PHYSICS-BASED AND DATA-DRIVEN MODELS USING A LOCALISED TRUSTWORTHINESS METRIC

Lars Bogaerts[1,2], Augustin Persoons[1,2], Matthias Faes[3] and David Moens[1,2]*

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ABSTRACT

Artificial Neural Networks (ANNs) can solve many (un)supervised learning tasks by virtue of the universal approximation theorem. In the context of on-line process control for manufacturing processes, ANNs are an ideal approach for e.g., on-line monitoring or prediction tasks. However, since they are trained on experimental input-output pairs, the governing physical relations are only implicitly included. This, for instance, can cause inaccuracies when extrapolating to out-of-sample data points. On the other hand, the numerical approximation of the governing physical laws via numerical methods holds strong potential for the accurate simulation of physical phenomena that occur during manufacturing processes. However, the corresponding computational effort is an impediment that arises with the need for numerous simulations [1]. This makes the application of such numerical schemes computationally intractable within an on-line monitoring context. As such, it is clear that ANNs and numerical simulation models have strong potential, but are fundamentally different models. However, their combination serves as a potentially efficient and accurate aggregated predictor, the so called grey box model. Such grey box model is based on highly efficient machine learning algorithms, the black box member, and backed by validated data with respect to physics generated by the numerical model, the white box member. A grey box model capable of defining a trustworthy prediction, including a measurement of uncertainty on the estimator, remains a challenging research topic.
In this paper, we introduce an ensemble machine learning method based on the residual modelling approach [2] that is able to provide a best-estimate under scarce data. We do so by combining the predictions of the white box, stemming from partial differential equations implemented in a multi-physics numerical solver, with the black box, representing the residual error between the white-box predictions and available experimental data. The novelty of this work is in the contribution of each counterpart in the grey box. The weight of each counterpart is based on distance metrics between available data in each model. We use real data sample points, generated by an experimental resistance pressure welding process to demonstrate that the proposed technique has a mean-squared error that is up to a constant lower than the error of corresponding estimators based on existing machine learning algorithms.

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Mathematics and algorithms for predictive digital twins (DT)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ENABLING TABULATED FLAMELET PROGRESS VARIABLE METHODS TO SOLVE THE REACTING NAVIER-STOKES EQUATIONS ON MULTIPLE ARCHITECTURES

Brian Bojko[1], David Kessler[1], Kamal Viswanath[1], Ryan Johnson[1], Andrew Kercher[1] and Andrew Corrigan[1]*

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ABSTRACT

The partial differential equations used to describe the reacting Navier-Stokes equations scale with the number of species being transported. This increases the numerical burden when solving combustion simulations using large reaction mechanisms that model real-world fuels of interest. Aside from the additional transport equations, numerical stiffness is also introduced into the system as different reaction rates progress on various time-scales throughout the domain. One method to increase computational efficiency and maintain a detailed description of the combustion physics is to utilize a flamelet progress variable (FPV) approach. The FPV approach reduces the number of species transport equations from N-1, N being the number of species, to three transport equations. In a diffusion flame scenario, the transported scalar quantities of mixture fraction (Z), reaction progress variable (Cpv), and mixture fraction variance (Zv) replace the species transport equations and fully describe the thermochemical state of the mixture. This method has been previously applied to multi-phase combustion phenomena of a reacting interface and extended to multi-phase spray flame configurations. A downside of the FPV approach for large combustion mechanisms, is the need to store large data tables which are loaded onto memory during simulations. This can potentially limit the number of species that can be cataloged in the table used to store the information, defeating some of the draw of this approach. Recent developments will be discussed on the use of a FPV dynamic source term and total energy transport approach to limit the need for multiple independent variables by decoupling the progress variable source term from the tables. Additionally multiple methods, including artificial neural networks (ANNs) will be discussed as a means of enable graphical processing unit (GPUs) for conducting simulations by reducing the memory storage of tables from the order of GBs to KBs. The FPV approach will be compared to the full reacting Navier-Stokes equations with detailed finite-rate chemical kinetics on multiple architectures for a set of canonical flames.

A HIGH-ORDER FLUX RECONSTRUCTION FRAMEWORK FOR INCOMPRESSIBLE FLOWS ON DEFORMING DOMAINS

Marie-Pier Bolduc[1] and Brian Vermeire*[1]

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ABSTRACT

A wide range of applications require accurate, efficient, and stable solution of incompressible flows around complex deforming geometries. For example, bio-flows, aerodynamics, and hydrodynamics. These prove challenging due to large deformations and intermittent flow separation, requiring unsteady scale-resolving solution techniques, Specifically Large Eddy Simulation (LES) and Direct Numerical Simulation (DNS).

Conventional computational frameworks rely on low-order finite volume methods, which require a prohibitively large number of degrees of freedom to resolve a range of turbulent length scales. Furthermore, enforcing incompressibility constraints typically relies on either exact incompressibility, via coupled global non-linear solvers, or artificial compressibility, via a number of pseudo iterations. Hence, performing scale-resolving simulations of incompressible flows on deforming domains is computationally expensive.

In this presentation, we will outline a novel high-order framework for incompressible LES/DNS flows on deforming domains. This framework utilizes the high-order flux reconstruction approach, enabling arbitrarily high-order accuracy on mixed-element unstructured meshes, combined with the Entropically Damped Artificial Compressibility (EDAC) method, weakly enforcing incompressibility without global solvers or pseudo stepping. Primary focus will be placed on the role of free stream preservation, order of accuracy preservation, enforcement of incompressibility constraints, and sub grid scale modelling via Implicit LES (ILES).

Numerical results will include canonical flows, such as the Taylor-Green vortex and turbulent channel flow, and practical industrial flows including moderate Reynolds airfoils, wing tip vortices, dynamic stall, and cardiovascular flows for the design of ventricular assist devices. These results demonstrate that the proposed framework maintains high-order accuracy, free stream preservation, enforces incompressibility, and is suitable for LES/DNS on deforming domains for a range of practical applications.

BAYESIAN SYMBOLIC REGRESSION: ADDRESSING CHALLENGES IN ESTIMATING FRACTIONAL BAYES FACTORS AND APPLICATION TO FATIGUE CRACK GROWTH MODELING

Geoffrey Bomarito[*1], Patrick Leser[1], Paul Leser[1] and Heather Hickman[1]*

[1]*NASA*

ABSTRACT

This research pioneers advancements in computational mechanics by integrating Bayesian-based uncertainty quantification into symbolic regression, specifically focusing on the critical task of accurately estimating the fractional Bayes factor for selecting arbitrary equations. In our exploration, we rigorously study two prominent methods—sequential Monte Carlo and the Laplace approximation—employed for computing the fractional Bayes factor.

Our findings underscore the limitations of the Laplace approximation, revealing its diminished accuracy in nonlinear and multimodal scenarios. Specifically, the Laplace approximation is shown to underpredict fractional Bayes factor on a wide set of equations associated with a symbolic regression benchmark. This comparative analysis sheds light on the nuanced performance of these techniques, guiding researchers toward more informed choices in uncertainty quantification within symbolic regression. Furthermore, we showcase the practical utility of these enhanced symbolic regression tools through their application to a real-world problem in fatigue crack growth modeling, emphasizing their efficacy in capturing the complexities of mechanical systems.

Contact and interface mechanics: Modeling and computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN ENERGY-CONSISTENT DISCRETIZATION OF HYPER-VISCOELASTIC CONTACT MODELS FOR SOFT TISSUES

*Francesco Bonaldi**[1], Mikaël Barboteu[1], Serge Dumont[1] and Christina Mahmoud[2]*

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ABSTRACT

We propose a mathematical model of hyper-viscoelastic problems applied to soft biological tissues, along with an energy-consistent numerical approximation. We first present the general problem in a dynamic regime, with certain types of dissipative constitutive assumptions. We then provide a numerical approximation of this problem, with the main objective of respecting energy consistency during contact in adequacy with the continuous framework. Given the presence of friction or viscosity, a dissipation of mechanical energy is expected. Moreover, we are interested in the numerical simulation of the non-smooth and non-linear problem considered, and more particularly in the optimization of Newton's semi-smooth method and Primal Dual Active Set (PDAS) approaches. Finally, we test such numerical schemes on academic and real-life scenarios, the latter representing the contact deployment of a stainless-steel stent in an arterial tissue. This is a joint work with Mikaël Barboteu, Serge Dumont, and Christina Mahmoud.

Multiphysics and data-driven modeling for cardiovascular biomedicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING THE HEMODYNAMIC IMPACT OF AORTIC ROOT ENLARGEMENTS IN AORTIC VALVE REPLACEMENT

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ABSTRACT

Surgical aortic valve replacement (SAVR) is the most effective treatment for patients with severe aortic stenosis (AS). However, patient-prosthesis mismatch is prevalent in up to 80% of cases and can lead to left ventricular hypertrophy and diastolic heart failure.[1] Aortic root enlargement (ARE) allows the implantation of larger valves, decreasing pressure gradients while providing a larger annulus for potential future transcatheter AVR (TAVR).[2] However, it has been suggested that ARE may also increase the risk of hemostasis and thrombus formation. In this study, we use computational modeling to understand the impact of an ARE on hemodynamics, assessing AV transvalvular pressure gradients, peak velocities, and hemostasis through residence times.

To assess the hemodynamic impact of ARE, we performed patient-specific CFD analysis of 4 pairs of matched AS patients. Each pair consists of a AVR+ARE patient matched with a AVR-no-ARE patient based on age, sex, ejection fraction, and native annulus size. For each AVR+ARE patient, we virtually deployed a SAV into their pre-operative geometry to act as another control model (virtual-AVR-no-ARE). These models provide a mechanism to assess hemodynamics across treatment strategies. Hemodynamic parameters, including heart rate and stroke volume, were standardized for all patients to isolate the effects of root anatomy. The 3D models are coupled to 2-element Windkessel models at the coronary arteries and aortic outflow and CFD simulations were performed on the finite-element multiphysics solver Cheart.[3] Transvalvular peak velocities and pressure gradients were calculated, and blood residence time was computed over 5 cardiac cycles.

AVR+ARE decreased the mean AV pressure gradient by 507% and 542% relative to the AVR-no-ARE and virtual-AVR-no-ARE matched controls. It also decreased the peak velocity by 74% and 56% relative to the AVR-no-ARE and virtual-AVR-no-ARE models. There was less than a 2.7% difference in blood residence time and all models had complete blood washout within 5 cardiac cycles. Hemodynamic simulations of AVR+ARE showed an expected marked reduction in the pressure gradients and peak velocity. Importantly, this came with only a minimal difference in blood stasis in the sinuses, suggesting a limited risk of thrombosis with ARE. Furthermore, the ARE procedure, followed by a simulated valve-in-valve, showed better hemodynamic outcomes over cases without enlargement, highlighting the long-term benefits of ARE.

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EFFECTIVE ELASTIC AND VISCOELASTIC PROPERTIES OF TUBULAR-ARCHITECTURED MATERIALS: ANALYTICAL AND NUMERICAL SIMULATIONS

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ABSTRACT

Several biological materials, such as bighorn sheep horns, hooves and human teeth, have the same micromechanical structure formed by neatly arranged tiny tubes. This microstructure is called tubular architecture and such natural materials generally exhibit ductility, high strength, impact and puncture resistance. This observation has attracted scholars to investigate the mechanical behavior of bioinspired structural materials with such microstructure. In this work, the effective elastic and viscoelastic properties of the material with tubular architecture, which were called tubular materials hereafter, were studied. The unit cell method was implemented in conjunction with an analytical solution and finite element simulations. Specifically, the analytical solution of the effective Young's and shear modulus in the displacement field was derived taking into consideration the state of the tubular material as a two-dimensional plane strain problem. Based on the analytical solution of the effective elastic moduli, the influence of the matrix properties on the tubular material, with different dimensions of normal circular or square holes distributed internally, was firstly investigated. Secondly, the relationships between the elastic moduli of the tubular materials and their corresponding volume fraction of holes were studied. The size effect of the tubular material in terms of relative density was also analyzed. On the other hand, the viscoelastic relaxation and creep response of the tubular materials were gained with aid of the same analytical theory and finite-element simulations. This fact has enabled us to obtain the viscoelastic model of the tubular material and then explore its time-dependent behavior under various loading paths and relative densities. By comparing the finite-element results with those obtained by the analytical solution, both effective elastic moduli showed a tendency to converge under higher deformations while, focusing on the size effect, their trend changed nonlinearly with the variation of the relative density in the displacement field. Moreover, changing the dimension of the normal holes, different variations in the time-dependent relaxation and creep responses of the tubular material were observed.

New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THERMOMECHANICAL TOPOLOGY OPTIMIZATION OF ROVER CHASSIS UNDER EXTREME CONDITIONS WITH BUCKLING LOAD CONSTRAINTS

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ABSTRACT

This study addresses level-set topology optimization of a rover chassis subjected to both thermal and mechanical loads with buckling constraints. The critical context of this research lies in the demanding conditions of space missions, where the equipment faces extremely low temperatures. The rover is also subjected to an exceedingly high range of temperatures, which leads to non-uniform material properties like coefficient of expansion throughout the domain. Maintaining the operational temperature range of this equipment necessitates a substantial amount of energy, which, if conserved, could be allocated towards enhancing instrument functionality for a more efficient mission outcome. Therefore, a key focus of this investigation is to develop a rover chassis that is not only structurally sound and thermally efficient but also lightweight, with a stringent volume fraction requirement of less than 5%. Topology optimization problems associated with low target volume fractions often result in designs featuring thin members prone to buckling. To ensure the stability of the optimized structure, one common approach involves conducting an eigenvalue analysis and imposing a lower limit constraint on the minimum buckling load. This ensures that the resulting design not only adheres to volume fraction limitations but also exhibits stability against buckling. The primary objective of our optimization problem is to minimize structural compliance, thereby enhancing the overall efficiency of the rover chassis. To meet the design goals, specific constraints are applied to volume fraction and minimum buckling load. Additional constraints on criteria like mean temperature are also considered. By incorporating these constraints, we ensure a holistic approach to the optimization problem, accounting for both structural integrity and thermal performance. A modular framework is developed that enables the implementation of multiple constraints and is compatible with legacy and/or open-source solvers and optimizers. For this work, PETSc and SLEPc libraries are used to implement linear boundary value problem solver and eigenvalue solver respectively.

Computational mechanobiology of musculoskeletal tissues
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMMBINI: A NOVEL IN SILICO APPROACH TO STUDY MECHANO-BIOLOGICAL REGULATION OF INFLAMMATION IN BONE FRACTURE HEALING

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ABSTRACT

Bone fracture healing is a convoluted process that involves many biological and mechanical factors working at different time- and length-scales. In the last decades, the investigation of this process has taken advantage of computer methods to simulate the hidden multiscale interactions which are challenging to explore experimentally. The initial inflammatory stage is rarely included in those computer studies of bone fracture healing [1]. With COMMBINI (Computational Model of Macrophage dynamics in the Bone Injury Immunoresponse) we filled this gap by using a hybrid modeling methodology that combines finite element analysis and agent-based models to simulate the mechanical and biological dynamics, respectively. To date, the biological part of COMMBINI has been developed for a standardized fracture set-up of a 0.7 mm fracture in mice tibia [2]. The interactions between immune cells and inflammatory cytokines have been simulated within the agent-based model to predict their spatio-temporal evolution during the inflammatory stage. The model has been parametrically calibrated and its results have been validated with a dedicated in vivo experiment [2]. The results highlighted the necessity to use the computational approach to have a more complete knowledge base of the numerous processes that regulate the process, which cannot be readily explained by experiments performed on immune cell cultures alone. For example, the model showed that a more realistic scenario, in line with in vivo macroscopic observation, has been captured when a macrophage proliferation rate was used that was higher than that reported from (in vitro) experiments [2]. Currently, the biological model of COMMBINI will be coupled with a finite element model to simulate the role of murine gait mechanics as the inflammatory stage of bone healing has been observed to be sensitive to mechanics [3]. The model will be extended to 3D and the macrophage regulation will be further influenced by mechanical cues. Macrophage mechano-regulation rules will be experimentally tested with dedicated macrophage-on-chip experiments under different user-defined mechanical conditions and implemented in COMMBINI. The overall model will be validated under alternative mechanical conditions with in vivo experiments on murine tibia stabilized with fixators of different rigidity. Once the model is validated and translated to the clinical sphere, it will provide the possibility to preliminary evaluate the rightful mechano-biological therapies to treat an injured patient, supporting bone healing from the initial inflammatory stage onwards.

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Fracture, damage and failure mechanics of cementitious materials
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CHEMO-MECHANICAL MODELLING OF BIOGENIC SULFIDE CORROSION OF CONCRETE

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ABSTRACT

This study presents a chemo-mechanical model for simulating biogenic sulfide corrosion in concrete sewer pipes [1]. The chemical model is based on a system of coupled diffusion-reaction equations that describe the processes of calcium hydroxide dissolution, calcium silicate hydrate dissolution, and gypsum formation. The chemical problem is two-way coupled with a mechanical model that captures the damage processes caused by mechanical deformations, calcium silicate hydrate dissolution, and gypsum formation. Numerical analyses demonstrate that the model realistically simulates the growth of a gypsum corrosion layer and the consequent damage development in the concrete material in in-situ sewer pipes. Validation experiments finally confirm that the chemo-mechanical model adequately simulates the shape of the experimental corrosion profile and the square root time development of the corrosion depth.

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Physical models and reduced order models augmentation with data for physics-informed machine learning in real-world applications
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OPERATOR LEARNING VIA NEURAL NETWORKS WITH KERNEL-WEIGHTED CORRECTIVE RESIDUALS

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ABSTRACT

Over the past few years, a novel class of methods known as physics-informed machine learning (PIML) has emerged as a promising alternative to traditional numerical methods for solving partial differential equations (PDEs). These PIML models typically rely on variants of neural networks (NNs) or kernel methods such as Gaussian Processes (GPs). In this presentation, we introduce NNs with kernel-weighted corrective residuals (CoRes, https://arxiv.org/abs/2401.03492) which integrate the best of both worlds: the scalability and extrapolation power of NNs with the superior local generalization properties of kernel methods. We demonstrate that our approach can (1) exactly satisfy the prescribed boundary and initial conditions, thereby simplifying the optimization process, (2) address inverse problems by incorporating additional measurements in the kernel structure, and (3) solve complex PDEs such as the Navier-Stokes equations as well as operator learning tasks. Through a diverse set of benchmarks, we show that our framework consistently outperforms state-of-the-art PIML methods in terms of accuracy, robustness and development time.

Smart structures – Modelling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SIMULATION AND ANALYSIS OF FUNDAMENTAL ORIGAMI FOLDING PATTERNS FOR DEPLOYABLE STRUCTURES

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ABSTRACT

Deployable structures are increasingly used in engineering and architecture, driven by the need for transportable and adaptable designs. Inspired by origami, the traditional art of paper folding, innovations arise in various fields such as micro and nanoscale systems, architected materials, biomedical applications, origami robots, reconfigurable structures for space exploration, and temporary settlements. The understanding of origami from mathematical models and the growing interest in computer-aided design have enabled the creation, analysis, and simulation of these foldable structures. This research focuses on simulating the behaviour of some fundamental origami patterns—Yoshimura, Miura, Waterbomb, Kresling, and Resch. This delves into the geometric properties, actuation forces, stresses, and deformations of these origami pattern. By simulating and comparing with physical models, we gain insights of how various origami patterns behave under different conditions and can estimate parameters such as folding ratio and useful volume. This comprehension of origami's basic units is key to selecting the most suitable patterns for the development of complex and space-efficient structures. The study can lead to the application of these patterns in practical scenarios such as origami-based deployable habitats, targeting key challenges in transportability, stability, and human safety, especially in extreme environments on Earth and space missions.

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A NOVEL ATRIAL-SPECIFIC IONIC MODEL FOR STEM CELLS-DERIVED CMS

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ABSTRACT

Human induced pluripotent stem cells-derived cardiomyocytes (hiPSC-CMs) have revolutionized the field of regenerative medicine, offering unparalleled potential for in-vitro modeling of normal and pathological human cardiomyocytes(1). The ability to produce stem cardiac myocytes in abundance has opened new avenues for drug efficacy and safety testing. The development of atrial fibrillation, for instanace, is influenced by ion channel mutations, genetic variants, and other risk factors. hiPSC-CMs hold promise in personalized medicine, as they share the genetic heritage of the donor.

In recent years, mathematical models of the ionic currents through the hiPSC-CM's membrane have focused on immature phenotypes, developing a system of stiff ordinary differential equations (ODEs). Previous studies characterizations of the CM's phenotype were based on action potential (AP) morphology, but the classification criteria were still undefined. Thus, the forerunner Paci2013(2) model was based on recordings obtained from a mixture of ventricular-like (VL), atrial-like (AL), and nodal-like hiPSC-CMs and the phenotypical heterogeneity was reproduced considering different scalings, instead of phenotype-specific currents.

Nowadays, the employment of electronic maturation highlights the chamber-specific AP phenotype of the cells and a phenotype-specific in-silico model is needed. In this direction, the latest version Paci2020 provides a developed ventricular-specific model. In this talk, I will present the first atrial-specific in-silico model of the hiPSC-CM ionic currents, based on experimental data provided by Altomare et al. Starting form an updated version of the ventricular Paci2020 model for AL hiPSC-CM, we incorporated the atrial-specific IKur and IKCa currents and a different IK1 formulation, inspired by the Koivumaki 2014 model of human adult atrial CM. Thus, the fine tuning of the model parameters was performed by means of an automatic optimization technique, in order to reproduce realistic AP transient shape and to speed up the parameter tuning phase(3).

The resulting model accurately reflects the experimental rate dependence data and demonstrates the expected response to a specific current blocker.

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A HU-WASHIZU STABILIZATION-FREE VIRTUAL ELEMENT METHOD FOR THREE- DIMENSIONAL LINEAR ELASTICITY WITH STAR-CONVEX POLYHEDRONS

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ABSTRACT

Numerical simulation of structures is a major pillar of industrial development. Indeed, numerical tools are used in very early stages of product development in order to achieve solutions that meet specifications as quickly and cost-effectively as possible. To meet growing industrial demand, we need to develop fast, robust numerical solvers. This calls for the development of new simulation methods such as the Virtual Element Method (VEM) which offers a very interesting framework to tackle common industrial issues such as mesh coarsening, node compatibility at contact interface and parallel mesh-generation on complex geometries.

Until the very recent work presented by [1], three-dimensional Virtual Element formulations required numerical stabilization terms to avoid the apparition of hourglass modes. Therefore, this study builds upon the recent developments on two-dimensional
stabilization-free Virtual Element formulations to introduce a stabilization-free Virtual Element Method for three-dimensional linear elasticity. To this end, a Hu-Washizu variational approach such as the one presented by [2] is used to define the weak forms of the equilibrium, compatibility, and constitutive laws in a three-field paradigm. The space for the independent strain field is then chosen to ensure the correct order of singularity of the local stiffness matrix. Finally, in this approach, the computation of the forementioned
matrix is done by the mean of additional degrees of freedom and carefully chosen projections.

The developed three-dimensional stabilization-free Virtual Element formulation have been tested on benchmark problems as well as in industrial contexts. Star-convex polyhedrons with planar faces have been used for meshing and the results shows robustness of the formulation including in the case of non-convex element geometry.

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Current trends in phase-field modeling and computations
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STATISTICAL MECHANICS-BASED GRADIENT-ENHANCED DAMAGE FOR ELASTOMERIC MATERIALS

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ABSTRACT

To design increasingly tough, resilient, and fatigue-resistant elastomers, a detailed understanding of the underlying damage cascade that leads to fracture needs to be found. To that end, we propose a statistical-mechanics based gradient-enhanced damage model for elastomeric materials and discuss the benefits and drawbacks between selecting a gradient enhanced damage approach and a phase field approach towards tackling this problem. The phase field fracture model has emerged as a popular computational method to study the fracture behavior of elastomers. In phase field fracture, a sharp crack is regularized via a diffuse crack phase field variable that minimizes the total potential energy of the system accounting for the (known) energy per unit cracked area for the specific material. Notably, the regularization length, functional form of damage modulation, and fracture toughness of the material must all be prescribed as model inputs in phase field fracture. However, the connection between essential network-level model components to fundamental polymer chain statistical mechanics has yet to be established, as the Lake and Thomas model is known to overestimate the fracture toughness and recent experiments by Slootman et al. (2020) have shown that chain scission can be physically delocalized away from the crack surface during the fracture process in elastomers. In this vein, an anisotropic stress-based gradient-enhanced continuum damage model grounded in elastomer statistical mechanics is formulated. Polydisperse elastomer chains are described by a statistical mechanics-based and thermodynamically-consistent polymer chain model accounting for bond extensibility. Chain scission and its corresponding dissipated energy are calculated via the principles of mechanochemistry. The non-local aspect of the model accounts for network level effects that influence the damage and fracture response connecting directly to a chain level damage criterion which is well established. This allows for fracture toughness to be recovered from our model, contrary to the phase field model where it would have to serve as an input. This is exceedingly important as one has to inherently consider rate dependence for the chain level rupture response. Furthermore, an imperfection sensitivity analysis is performed, connecting the non-local interaction length, introduced in this modeling framework, to the fractocohesive length scale.

Next-generation numerical methods for coupled multiphysics problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COUPLED MULTIPHYSICS SIMULATIONS FOR HIGH ENERGY DENSITY PROBLEMS

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ABSTRACT

Research to understand high energy density physics (HEDP) phenomena is often conducted using pulsed power machines that are capable of producing powerful bursts of energy in a very short time. Particle accelerators, lasers, ITER and other devices such as National Ignition Facility (NIF) at Lawrence Livermore National Labs (LLNL) and Z machine at Sandia National Labs (SNL) are the examples. Energy is typically produced in the form of a particle beam or burst of radiation of the various spectra, from thermal to visible light to X-rays, which is directed towards target being studied, but is also absorbed by the components of the machine, measurement devices and other equipment. Sudden deposition of that energy can result in rapid local heating of the materials, followed by expansion and, if sufficient amount of energy is absorbed, ablation of the thin layer of the material. Both phenomena result in stress waves that propagate through potentially sensitive equipment.

Understanding of this phenomenon is necessary for proper design and safe and reliable operation of the pulsed power machines and measurement devices used in the experiments, yet complexity of the physics involved makes prediction of such behavior difficult. Different temporal and geometric scales present in the problem only further complicate things.

To address this problem we developed two step simulation approach where physics associated with energy deposition (very short duration and small dimensions) is modeled using multiphysics Arbitrary Lagrangian-Eulerian (ALE) code ALEGRA followed by structural analysis on typical structural and temporal scales using SIERRA/SM. Both codes have been developed at the SNL. Different temporal and spatial scales allow to use simple one way coupling between the codes by initiation of structural analysis using results of the multiphysics simulation.

In our presentation we will describe details of both problems formulations and explore different ways of coupling of the two models, discuss pitfalls and advantages of the approach and evaluate accuracy of the different ways performing simulations.

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Advanced model order reduction techniques for computational fluid dynamics
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EXPLORING HIGH-DIMENSIONAL TURBULENT DYNAMICAL SYSTEMS WITH AUTOENCODERS

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ABSTRACT

We investigate the exploration of high-dimensional dynamical systems, following incompressible Navier-Stokes equations in the turbulent regime, using Machine Learning (ML) dimension reduction techniques. We will review recent methods based on different AutoEncoders (AEs) to efficiently analyze and understand turbulence through dimensionality reduction. The primary objective is to employ AEs architectures to find a parametrisation of the large phase space expressed in a lower-dimensional representation, unraveling key variables of the flow. Essentially, AE-methods map the system phase space to a sub-space (called latent space) and back, by optimizing two large parametric transformation functions (Neural Networks) through gradient descent. If this optimisation process converges, it means that some redundancy, correlations, or symmetries allow a dimension reduction without loss of information.

Recent work have taken advantages of different AE architectures to highlight some general properties that need to be enforced in the model architecture or at the optimisation level [1], to better capture non-linearity of the system phase space. While further advances are needed to model with robustness the system trajectory in the latent space, due to chaos, it remains possible to sample accurately the flow steady state in the long run [2]. Overall, the last decade has shown that ML methods like AEs perform at least an order of magnitude better than classical linear methods, such as Proper Othogonal Decomposition (POD) and Dynamical Mode Decomposition (DMD). The use of AE-based methods for dimension reduction offers a promising avenue for Reduced Order Modelling (ROM) of turbulent flow.

Our contribution beyond previous work will be to propose new Machine Learning metrics, based on the sub-space statistical distributions and correlations in a data augmentation setup, to constraint the latent space local geometry and symmetry. The method is showcased on the von Kármán turbulent flow [3]. The aim is to characterize precisely system trajectories in the latent space and better estimate the turbulent attractor dimension, and dynamic at play.

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Computational modeling of extreme-loading events
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE MODELING OF THE BALLISTIC PERFORMANCE OF UNCONFINED AND CONFINED POLYMERS

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ABSTRACT

Due to their high strain rate dependence and high specific energy dissipation, polymers and polymer composites are good candidates for advanced lightweight protection against high velocity impacts and shocks. Confinement has been shown to play an important role in enhancing the performance of certain ballistic resistant materials (such as concrete and ceramics). However, less is known about the effects of confinement on the response of polymers, especially during ballistic impact. Polymers under confinement exhibit notable changes to their molecular structure and material properties as the free space between polymer chains is reduced. Reduced free volume leads to higher interchain friction, which increases strength and stiffness and can provide enhanced energy dissipation. In this work, molecular dynamics (MD) and finite element (FE) simulations are conducted to investigate the multiscale ballistic performance of a ductile polymer with and without confinement. For the unconfined polymer, the energy absorbed (EA) per unit mass predicted through MD simulations is shown to scale well from the nanoscale to the macroscale, matching closely with predictions from macroscale FE simulations of ballistic impact. Under the confinement of a thin graphene backing plate, ballistic MD simulations exhibit drastic increases in the amount of EA due to enhanced interchain friction. Macroscale FE simulations predict a smaller EA increase due to confinement compared to the nanoscale, suggesting that size scale could play an important role in understanding confinement effects in polymers.

Applications of shape optimization in complex engineering problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFICIENT AND FLEXIBLE SHAPE SENSITIVITY CALCULATIONS FOR FINITE ELEMENT METHODS VIA AUTOMATIC DIFFERENTIATION

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ABSTRACT

Direct optimization of the nodal positions in a computational mesh in conjunction with various filtering schemes is a promising methodology in shape optimization [3]. To support these methods, analysis schemes with derivatives with respect to nodal coordinates are needed. These derivatives are often difficult to calculate and require either complex manual derivation or inaccurate finite difference techniques.

In this talk, we outline a new framework used to calculate these derivatives flexibly and efficiently. On top of the reference finite element mesh, we define a new shape displacement field that translates the reference coordinates to their new optimized location. This field is discretized using standard finite element basis functions and can now be interpolated at quadrature points. We exploit the structure of the finite element method to efficiently calculate sensitivities of the finite element residual with respect to this shape displacement field via forward-mode automatic differentiation at each quadrature point. Once these modifications to the shape field are made, we expose the quadrature point functions directly to the user. This enables rapid development of novel nonlinear shape optimization problems within an HPC-ready code. We describe the implementation of this methodology in Serac [2], an open-source thermomechanical simulation engine built on the MFEM finite element framework [1]. Finally, we conclude with some current applications of our code including sensitivity analysis of nonlinear responsive liquid crystal elastomer structures and porous electrodes.

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Modeling and simulation of dynamics, stability and control of aerospace structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL AND EXPERIMENTAL ANALYSIS OF THE EFFECT OF GEOMETRIC NONLINEARITY ON AEROSPACE STRUCTURES SUPPORTING NON-IDEAL ROTATING MACHINES

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ABSTRACT

We present a numerical and experimental study of the effects of geometric nonlinearities on vibrations of rotating machines aerospace slender support structures. The initial stiffness of a structure, computed in its unloaded state, is affected by the applied forces, the so-called geometric stiffness. Here we study these effects via numerical and experimental methods designed to evaluate previous mathematical models. Our model is a slender three members metal portal frame, under compression of its columns and beam, supporting a non-ideal rotating machine. The presence of large axial compressive force will reduce the structure's stiffness and natural frequencies, leading to unexpected, potentially dangerous, resonance states. Experimental imperfections led to observation of interesting phenomena not predicted in our previous theoretical and numerical studies. We also observe, as expected, occurrence of the so called Sommerfeld Effect, when underpowered excitation sources get their rotation regime stuck at resonances and are subjected to jump phenomena.

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Biomechanics of hard tissues: From experiments and simulations to clinical applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BIOMECHANIC SIMULATIONS OF FRACTURE NON-UNIONS CAN DETERMINE THE NEED TO ADDRESS OSTEOSYNTHESIS STABILITY DURING REVISION SURGERY – A CLINICAL STUDY AND FINITE ELEMENT ANALYSIS

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ABSTRACT

Introduction
Fracture non-unions are associated with a high burden of disease. The two main determinants of non-union outside of infected situations are biology and local mechanics. Aim of this study was to test the capability of our in vivo simulation workflow to calculate the mechanical environment of a non-union situation pre and post revision surgery, determine the mechanical adequacy of the treatments and compare the simulation results to the healing course of the patient.

Methods
In a clinical case series of non-union patients requiring operative revisions a musculoskeletal simulation was performed. Clinical CT imaging was used to construct a three-dimensional CAD-model of the treatment situation before and after non-union revision. Resulting forces are then computed in a simulation-driven workflow (Braun et al. Frontiers in Surgery 2021) based on motion capturing data. The forces are used to simulate the mechanical fracture environment. From the simulation implant stresses for the initial and revision situation, as well as interfragmentary movement and resulting strain are calculated and compared to the clinical course.

Results
Over 40 patients have been included to date in different non-union locations of the upper and lower extremity. The simulation workflow was able to calculate and visualize implant mechanics, interfragmentary strain and resulting tissue differentiation probability based on the Claes bone healing boundaries. The changes through implant revision could be accurately calculated. Especially in mechanically addressed hypertrophic non-union situations the mechanical changes in relation to fracture healing could be highlighted (Fig. 1).

Discussion/Conclusion
The presented workflow was able to visualize critical non-union mechanical conditions both pre and post revision surgery. Mechanical adequacy towards non-union healing can be calculated in relation to patient specific motion capturing. The simulation has the potential to help determine the most appropriate revision strategy in complex non-union situations.

Design and mechanics of mutifunctional composites and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPERIMENTAL ANALYSIS OF THE MECHANICAL PROPERTIES OF 3D PRINTED POLYMER COMPOSITE SPECIMENS

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ABSTRACT

Additive manufacturing (AM) technologies are defined according to ASTM standard f2792-12A [1] as a process in which materials are joined to produce objects from a 3D model. One of the most popular AM techniques is Fused Filament Fabrication (FFF), commonly known as 3D printing, which is classified as a material extrusion process because the material is applied through a nozzle or extruder. Several materials are the most popular filaments for 3D printing. These include polylactide or polylactic acid (PLA), acrylonitrile butadiene styrene (ABS) and acrylonitrile styrene acrylate (ASA). Recently, researchers have focused on investigating the mechanical properties of blends of several of these base materials. In this work, one such composite/blend is presented, namely a mixture of ABS and mainly thermoplastic polyurethane (TPU), with ABS serving as the matrix and TPU as the reinforcement, i.e. a composite material, as investigated in [2]. Several different infill patterns are considered, while all blend combinations having similar volume fractions. The basic mechanical properties are investigated and reported in the form of a stress – strain curve together with the modulus of elasticity. In addition, low-cycle fatigue (LCF) is investigated and performed as follows. Three different load percentages were considered, namely 50 %, 70 % and 90 % of the maximum tensile force, according to the results of the tensile tests. The threshold value for the number of cycles was set at 1000 cycles at a speed of 5 mm/min. If the specimen withstood 1000 cycles, the test was continued with the static tensile test until the specimen broke. The maximum force and maximum displacement were recorded. If the specimen did not withstand 1000 cycles, i.e. if the fracture occurred before the 1000 cycles were reached, the maximum number of cycles was recorded. Such a test method is proposed in [3] and was suitable as a reference method.

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Advances in material model calibration for computational solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN APPROACH INTEGRATING SIGNED DISTANCE FUNCTIONS WITH THE ADJOINT METHOD TO ESTIMATE TISSUE MATERIAL PROPERTIES USING CLINICAL IMAGING DATA

Elaheh Mehdizadeh[1], Amin Pourasghar[1], Timothy Wong[1], Arvind Hoskoppal[1] and John Brigham[1]*

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ABSTRACT

A computational method will be presented for estimating the spatial distribution of mechanical properties of soft tissues within the body, particularly the heart wall, using clinical imaging data. The core innovation lies in a newly devised shape-based approach that utilizes a signed distance function method to measure the difference between image-derived target and simulated tissue mechanical behaviors. This approach is an extension of prior work by the authors that used a standard discretized version of the Hausdorff distance as an objective function in an iterative approach to material parameter estimation [1]. As such, a novel level-set framework is introduced for the objective function that is differentiable and is implemented into an optimization framework to identify the material parameters that minimize the difference with respect to a “target” shape with relative computational efficiency. The adjoint method is employed to calculate the gradient throughout optimization, further enabling efficient minimization of the shape-based objective function. In additional to presenting the computational procedure, the method will be evaluated via simulated inverse problems based on estimating passive heart wall mechanical material properties from standard cardiac clinical imaging data and hemodynamics (i.e., intraventricular pressure). These computational tests consider a simplified system of a two-dimensional (slice) of the bi-ventricular wall with the diastolic process estimated by applying intraventricular pressure, and considers only elastic material properties. Assessment of the results will include the capability to minimize the shape-based objective function effectively and consistently, the accuracy of the estimated material parameters, and the effects of model error on the inverse solution estimation process. Longer-term objectives involve integrating the computational approach with more realistic in vivo conditions, including geometry and boundary conditions. Moreover, the approach will be extended to have the capability to estimate more generalized heterogenous properties and/or alternate constitutive models.

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Recent advances in high-order methods for computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NONLINEARLY STABLE HIGH-ORDER METHODS FOR WALL-BOUNDED FLOWS

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ABSTRACT

Following the work on viscous free shear flows [1] using the PHiLiP code [2], an assessment of large eddy simulation (LES) approaches for wall-bounded flows using nonlinearly stable flux reconstruction (NSFR) [2] is presented. For all approaches, the filtering is accomplished implicitly by using an under-resolved computational mesh. These implicitly filtered LES (iLES) approaches include: (1) wall-resolved iLES (WRiLES) without a sub-grid scale (SGS) model, (2) WRiLES with an SGS model, (3) wall-modelled iLES (WMiLES) without an SGS model, and (4) WMiLES with an SGS model. The performance of several different SGS models is assessed, including the: wall-adapting local eddy-viscosity (WALE) model, the Vreman model, the high-pass filtered Smagorinsky model, and the dynamic Smagorinsky model. In terms of the wall-models, we consider: (1) the analytical Reichardt law-of-the-wall, and (2) the ordinary differential equation (ODE) compressible equilibrium model. The assessment is performed using the canonical turbulent channel flow case. The findings of this study aim to answer several open research questions in regard to what the best LES strategy for simulating wall-bounded flows is when using a provably-robust high-order discretization scheme.

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Phase-field modeling: Analytics, benchmarks, and discussions
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHASE-FIELD MODELING AND EFFECTIVE SIMULATION OF NON-ISOTHERMAL REACTIVE TRANSPORT

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ABSTRACT

We consider non-isothermal single-phase flow with solute transport where ions in the fluid can precipitate and form a solid mineral, and where the mineral can dissolve and release solute into the fluid. The model is quasi-compressible, hence non-matching fluid and solid densities are allowed in the model formulation. The evolving fluid-solid interface is approximated by a conservative Allen-Cahn equation. This equation includes a non-local term, which makes the use of standard Newton iterations for solving the resulting non-linear system of equations inefficient. We instead apply L-scheme iterations, which are cheaper to perform and is proven to converge for any starting guess. However, L-scheme iterations give only linear convergence. The coupled equations for diffuse interface, solute transport and heat transport are solved via an iterative coupling scheme, which is proven to converge under mild restrictions on the time-step size and on an added regularization parameter. This coupling scheme allows the model equations to be solved more efficiently compared to a monolithic scheme, and numerical experiments show that only few iterations are needed to obtain high accuracy.

Part of this work is available in [1].

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Data science and machine learning applications for composite materials and biomedical engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VISCONET – A MACHINE LEARNING FRAMEWORK FOR POLYMER NANOCOMPOSITE VISCOELASTIC PROPERTY PREDICTION AND MATERIAL DESIGN

Catherine Brinson[*1], Anqi Claire Lin[1] and Richard J. Sheridan[1]*

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ABSTRACT

Polymer-based nanocomposites (PNCs) are formed by dispersing nanoparticles (NPs) within a polymer matrix, which creates polymer interphase regions that drive property enhancement. However, data-driven PNC design is challenging due to limited data and poor understanding of the impact of the interphase region. To address the challenge, we present ViscoNet, a surrogate model for finite element analysis (FEA) simulations of PNC viscoelastic (VE) response.

ViscoNet leverages the pre-training-then-fine-tuning training scheme, inspired by successful approaches used in the natural language processing (NLP) domain. Pre-training the model with a large dataset from finite element analysis (FEA) simulations covering a wide parameter space enables it to build a general understanding of VE response (see Figure). Subsequently, the model is finetuned with a smaller dataset specific to the materials system of interest, refining its knowledge for accurate material-specific predictions. We utilize a simple multilayer perceptron (MLP) architecture, offering fast training and inference times. To address the issue of reducing the VE response to an ANN input vector, we employ a frequency-fixing technique, transforming the 2D spectral response curve into a 1D series.

We explore ViscoNet's effectiveness through generalization tasks, both within qualitatively different thermoplastics and from thermoplastics to thermosets, reporting a mean absolute percentage error (MAPE) of < 5% for rubbery modulus and < 1% for glassy modulus in all cases and 1.22% on tan(δ) peak height prediction. With only 500 FEA simulations for finetuning, ViscoNet can generate over 20k VE responses within 2 minutes with 1 CPU, compared to 97 days with 4 CPUs via FEA simulations. This fast, low-resource, yet reliable approach significantly enhances the accessibility of data-driven materials design of PNCs, since neither cloud compute nor even GPU resources are required for fast training, fine-tuning, and inference. In a VE material design loop, ViscoNet will enable insights and discoveries by either replacing the FEA simulation component as a surrogate or fill the design space directly thanks to its lightning-fast inference speed.

By predicting the entire VE response, ViscoNet surpasses previous scalar-based surrogate models for FEA simulation, offering better fidelity and efficiency. The training data for ViscoNet is being curated into a materials repository, MaterialsMine, and ViscoNet will be made available as a tool on the MaterialsMine website for researchers to use.

Imaging and computational methods for biomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A PERSONALIZED MULTISCALE MODEL OF BIVENTRICULAR CARDIAC MECHANICS

Aaron Brown[*1], Lei Shi[2], Matteo Salvador[1], Fanwei Kong[1], Vijay Vedula[3] and Alison Marsden[1]*

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ABSTRACT

Numerical simulations of the biomechanics of the heart are useful for non-invasive investigations of cardiovascular disease mechanisms and treatments. In such simulations, modeling the circulatory system is essential for capturing physiological cardiac behavior. To reduce the computational cost, blood circulation is typically represented with a zero-dimensional (0D) lumped-parameter network (LPN). Recently, we described a novel scheme to couple three-dimensional (3D) cardiac mechanics models with 0D circulatory models, demonstrating the method with an idealized left ventricle coupled to an open-loop LPN. Here, we extend the coupling scheme to an image-derived, biomechanical model of the ventricles coupled to a closed-loop LPN, which is further personalized to clinical measurements.

Phase-resolved (3D+t) computerized tomography images are obtained for an adult male at 10 time points during the cardiac cycle. We then apply a deep-learning approach to segment the images [1] and calculate time-dependent cardiac chamber volumes. Other clinical measurements, including cuff blood pressures and electrocardiogram waveforms, are also obtained. For the ventricular myocardium, the equations of hyperelastodynamics, with the fiber-based Holzapfel-Ogden material law, are solved using a recent finite element method suitable for incompressible finite deformations [2]. The circulatory system is modeled using a closed-loop LPN. The two submodels –- 3D biventricular mechanics and 0D blood circulation –- are coupled using our recently published method [3]. To personalize the model to clinical measurements, we first tune the LPN parameters, then determine the stress-free configuration and passive material parameters of the myocardium, and finally optimize the parameters of the active contraction model.

This work provides a methodology and a baseline model for simulating personalized biventricular mechanics. Using a high-fidelity 3D model for the myocardium, but a simplified 0D circulation model, permits a physiological yet computationally tractable simulation of the heart function. Our preliminary results exhibit physiological cardiovascular behavior, including the downward motion of the atrioventricular plane, reasonable pressure-volume loops, and equalization of stroke volumes after several cardiac cycles. The isovolumic phases of the cardiac cycle, which traditionally pose numerical challenges, are captured by our coupling method without any ad hoc special treatment [3]. One can modify this model to investigate the effect of congenital heart defects, as well as surgical interventions to address such diseases. The method may also be extended to four-chamber heart models to simulate whole-heart cardiac mechanics.

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Computational fluid dynamics (CFD) and fluid-structure interaction (CFSI): Methods and Applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ACCURATE AND ROBUST MAPPING ALGORITHMS FOR GENERAL MULTI-PHYSICS COUPLING

David Brown[1], James Thunes[1] and Daniel Williams[1]*

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ABSTRACT

Mapping, in a multi-physics context, is the problem of transferring data from the source to target side of a geometric interface of two physics solvers. Accurate mapping technology is critical to any multi-physics coupling engine. Many technologies exist for accomplishing this, with various properties, often well-suited to particular applications, but often not well-suited to problems outside of their target application. One mapping technology in particular, radial basis functions (RBFs) , is a popular choice due to its wide applicability, requiring as input only points and data, thus being applicable to any type of source mesh or point cloud. Unfortunately, this approach frequently encounters pathologies depending on the particular RBF formulation and arrangement and profile of the source data. We encounter a wide range of source data profiles in real-world applications due to different interface topologies, which can be surface mesh, volume mesh, or point cloud; data location provided by the solver, which can be element centroid, integration point, or node; and different physics applications, which can affect the mesh profile as well as the profile of the source data itself . These different features can result in Runge phenomenon, poor conditioning of the RBF matrix, or even an ill-posed interpolation problem. It can be very challenging to design an accurate and reliable mapping algorithm for general applications.

The presentation will focus on new algorithms for mapping non-conservative data for real-world industrial multi-physics applications. The presentation will begin with a technical presentation of the interpolation problems targeted, and the general approach to the mapping. We demonstrate several pathologies encountered by standard RBF formulations in specific cases, their root causes, and new solutions to these problems. The proposed solutions include modification to the RBF formulation, pre- and post-processing techniques for source and target data, and a detection-correction approach to dimensionality reduction to avoid ill-posedness. We also present our analysis of the conditions needed to conserve the minimum order of accuracy of the coupled solvers, and demonstrate how this information can be used to develop a regularity-favorable source point cloud for the RBF algorithm.

The algorithms as described will be commercially available as part of the Ansys System Coupling version 2025R1 multi-physics engine.

Computational modeling of extreme-loading events
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SECOND-ORDER PYRAMIDS SUPPORTING EXPLICIT SOLID DYNAMICS FOR SIMULATION OF EXTREME EVENTS

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ABSTRACT

Explicit dynamic methods are frequently used to simulate extreme events, such as car crash and other severe impacts, as well as weapon effects and accidental explosions. Frequently, the structural geometry can be tedious to mesh, which has given rise to hex-dominant meshing algorithms. Leveraging such methods, however, typically requires the use of not only hexahedral (hex) and tetrahedral (tet) elements, but also transition elements providing compatible faces with each. When the parts being meshed contain curved edges and/or surfaces, second-order elements also become advantageous by allowing geometric features to be modeled more accurately with fewer elements. Such approaches have been more prevalent in implicit models, but are gaining attention in explicit methods. A key to successful hex-dominant meshing with second-order elements for explicit nonlinear solid dynamics, was the development of a robust 19-node pyramid element (PYR19), that is compatible with other robust second-order solid elements. The PYR19 has been shown to behave well in flexure with very few elements. It also resists volumetric locking in problems involving metal plasticity and shows no signs of hourglassing by virtue of its robust quadrature. The PYR19 and its compatible elements are available for use in parallel explicit solid mechanics codes. The elements are also supported in popular meshing and visualization software.

Data-driven methods for modeling complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LEVERAGING DATA AND THE KOOPMAN OPERATOR TO CONTROL SOFT ROBOTS

Daniel Bruder[*1]

[1]*University of Michigan*

ABSTRACT

Soft robots are able to safely interact with delicate objects, absorb impacts without damage, and adapt to the shape of their environment, making them ideal for applications that require safe robot-human interaction. However, their use in real-world applications has been limited due to the difficulty involved in modeling and controlling soft robotic systems. In this talk, I'll describe a modeling approach aimed at overcoming the limitations of previous methods. This data-driven approach leverages Koopman operator theory to construct models that are linear, which enables the utilization of linear control techniques for nonlinear dynamical systems like soft robots. Using this Koopman-based approach, a pneumatically actuated soft arm was able to autonomously perform manipulation tasks such as trajectory following and pick-and-place with a variable payload without undergoing any task-specific training. In the future, these approaches could offer a paradigm for designing and controlling all soft robotic systems, leading to their more widespread adoption in real-world applications.

Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL ANALYSIS OF DAMAGE AND FAILURE BEHAVIOR OF ANISOTROPIC ALUMINUM SHEETS UNDERGOING BIAXIAL LOADING

Michael Brünig[*1], *Sanjeev Koirala*[1] *and Steffen Gerke*[1]

[1]*University of the Bundeswehr Munich*

ABSTRACT

In the presentation the effect of stress state and loading direction with respect to the principal axes of anisotropy on damage and failure behavior of the anisotropic aluminium alloy EN AW-2017A is investigated. New experiments with biaxially loaded specimens and corresponding numerical simulations have been performed to develop a damage criterion and a damage rule predicting macroscopic strains caused by different damage mechanisms on the micro-level. During the tests digital image correlation is used to monitor evolution of strain fields in critical parts of the specimens. Failure modes on fracture surfaces are visualized by scanning electron microscopy. In addition, numerical calculations on the micro-level considering void-containing representative volume elements reveal further information on damage and failure processes. Based on the experimental data and numerical results of three-dimensionally loaded unit-cells damage laws depending on the stress state and on the loading direction are developed. They are validated by numerical simulation of the tests with biaxially loaded specimens showing good agreement of experimental and numerical results. It is shown that the stress state, the load ratio and the loading direction with respect to the principal axes of anisotropy have an influence on the width and the orientation of localized strain fields as well as on the formation of damage processes and fracture modes on the micro-scale.

Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ROBUST NUMERICS AND SUB-GRID MODELS FOR MULTI-PHYSICS CFD AT EXASCALE

Anand Radhakrishnan[1], Benjamin Wilfong[1] and Spencer Bryngelson[*1]*

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ABSTRACT

Multi-phase flows arise broadly, from cavitation around high-speed underwater vehicles to biomedical treatments for kidney stones. The combination of scales in these problems, and others like them, lead to simulations with large grid sizes and small time steps. Still, understanding multiphase flow phenomenologies and the quantities of interest that buttress them are required to develop sub-grid models for them, such as those of Euler-Euler and Euler-Lagrange types. This work presents the use of CFD software at exascale to conduct full-resolution simulation for computational modeling.

We show that exascale supercomputers, like OLCF Frontier, can enable unprecedented resolution and simulation of compressible multi-phase problems. These simulations are conducted via the Multi-component Flow Code (MFC; Bryngelson et al. Comp. Phys. Comm. (2021)). MFC is open-source and GPU-accelerated. The MFC solver uses high-order accurate numerics and marshals different multi-component diffuse interface (4-6 equation models) and sub-grid models for particles, bubbles, and droplets.

Efficient use of exascale systems requires performant numerics on NVIDIA- and AMD-GPU-based supercomputers. We accomplish this via high-order WENO reconstructions and HLL-type approximate Riemann solvers. Flux computations are dimensionally-split and array reshaping enables performant nested loop computation in the most expensive kernels: reconstructions and Riemann solves. These methods are offloaded to GPU devices via OpenACC, achieving about a 300-times speedup in the most expensive kernels over single CPU cores. Our combination of numerics and GPU acceleration has weak scale nearly ideally (within 95%) to all of Frontier, the first exascale GPU supercomputer (66K GPUs).

Multiscale computational and data-driven approach of advanced materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GRAPH NEURAL NETWORKS FOR 3D GEOMETRY-AGNOSTIC PREDICTIONS OF MATERIAL BEHAVIOR

Robert Buarque de Macedo[*1], Kevin Potter[1], Kyle Johnson[1] and Craig Hamel[1]*

[1]*Sandia National Laboratories*

ABSTRACT

The FEM (finite element method) has seen tremendous success in the last few decades for accurately modeling complex material behavior. However, simulations can become prohibitively computationally expensive for real-world use cases. This is particularly true when simulations must be run with a range of parameters. In recent years, surrogate modeling with neural networks has been researched to accelerate physics-based simulations. In this data-driven paradigm, networks are trained to predict the results of expensive FEM runs. Once trained, the networks can quickly forecast the simulation results in a fraction of the time, trading off accuracy for speed. In this work, we investigate a particular type of neural network – graph neural networks (GNNs) – as surrogate models for notoriously hard to capture geometries in solid mechanics FEM simulations. Unlike convolutional neural networks (CNNs), which assume a fixed-sized input and output across all data, GNNs process graph objects with arbitrary numbers of nodes and edges. As such, a GNN is “geometry agnostic”: it can input and output an FEM mesh rather than being constrained to predictions on fixed sized voxelated representations of models. We investigate the efficacy of GNNs as FEM surrogates for two use cases. First, we attempt to learn the behavior of porous metal microstructures. GNNs are used to predict the evolution of equivalent plastic strain in these domains. It is studied what features the GNNs can predict, and to what extent the graph connectivity and nodal values contribute to the predictions. Secondly, we apply GNNs towards estimating mechanical behavior of complex geometries such as fasteners. From these results, it is investigated how well GNNs can generalize across a range of geometries. This research represents a critical step in applying data-driven surrogate modeling towards general, complex 3D geometries of practical interest.

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16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Advances in discretization techniques, element technology, mesh adaptivity, and solution strategies for inelasticity, localization, and failure

July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PROGRESS AND CHALLENGES IN THE DEVELOPMENT OF THE COMPOSITE WEDGE LOCALIZATION ELEMENT

Michael Buche[1], Michael Veilleux[1], Ellen Wagman[1], John Emery[1], Alejandro Mota[1] and James Foulk[1]*

[1]*Sandia National Laboratories*

ABSTRACT

Localization elements were originally developed to regularize sub-grid localization processes occurring in finite element analyses while utilizing the same constitutive model as the bulk. The 10-noded composite tetrahedral element has been recently improved to provide accuracy under large isochoric deformations while enabling practical meshing. In order to extend the ductile failure capabilities of composite simplices to include strain localization and fracture, a 12-noded composite wedge localization element has been developed. The mathematical formulation of this element is a relatively complicated but direct combination of the 10-noded composite tetrahedral element and the original localization elements. As opposed to the original localization elements, which use a variational scheme to determine the localization length scale, here it is treated as a material parameter that can be calibrated to material properties like the fracture toughness. Recent progress in developing this composite wedge localization element includes the introduction of a second length scale to provide some stabilization through independent control of membrane forces. Ongoing work considers the possibility of in-plane locking and implementation of projection-stabilization strategies similar to the 10-noded composite tetrahedron, as well as pathologies that are unique to the 12-noded composite wedge localization element.

Data-driven device and circuits models
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN CIRCUIT-LEVEL RESPONSES TO DEVICE-LEVEL VARIATION VIA XYCE-PYMI

Paul Kuberry[1], Thomas Buchheit[1], Biliana Paskaleva[1], Andrea Jin[1], Ting Mei[1] and Coby Davis[1]*

[1]Sandia National Laboratories

ABSTRACT

Rapid generation of accurate electrical device models is important to many disciplines, including those tasked with quantifying the effects of aging on commercial off the shelf (COTS) components. Traditionally, compact device level models use idealized expressions for current and charge response of the device from an applied voltage. These models require subject matter experts with proprietary tools to perform calibration from collected data. Because there is no guarantee that the idealized expressions precisely represent the observed data, it is possible that even more time must be spent heuristically adding additional components to an existing model to achieve the desired fit. Certain classes of data-driven models allow for automated use of data collected in the field or laboratory, thus enabling rapid circuit level simulations. The modeling approach and workflow described in this presentation are demonstrated in the context of NPN bipolar junction transistors (BJT) in an LM741 operational amplifier for low frequency, non-capacitive regimes. We use Xyce-PyMi Python-based modeling interface to develop and evaluate our data-driven device models in a Xyce circuit simulator and use the Sandia Analysis Workbench (SAW) to capture and fully automate the entire process from data to circuit simulation. The successful implementation of the data-driven device and circuit levels modeling approach into a workflow sets the stage for continued development of data driven modeling into capacitive regimes and a wider range of devices, including MOSFETS. Both development extensions will be discussed in the presentation.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525.

Computational and analytical advances in nonlocal modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPARING TWO NONLOCAL BIHARMONIC OPERATORS

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ABSTRACT

Nonlocal operators are advantageous in modeling given their flexibility in handling discontinuities, incorporating nonlocal effects, and modeling a range of interactions through different choices for kernels. Using these operators in models has several applications, including peridynamics. The biharmonic operator appears in many models including deformations of beams and plates. The nonlocal biharmonic operator can be formulated in at least two ways: using a fourth difference operator or iterating the nonlocal Laplacian. In this talk, we discuss various aspects of the two operators, including convergence of the operators to their classical counterpart and requirements for asymptotically compatible schemes.

Continuum biomechanics of active systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFECT OF REGION-DEPENDENT MATERIAL PROPERTIES OF HUMAN BRAIN TISSUE DURING SURGICAL PROCEDURES

Emma Griffiths[1], Nina Reiter[1], Jan Hinrichsen[1], Jayaratnam Jayamohan[2] and Silvia Budday[1]*

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ABSTRACT

Accurate finite element models of the human brain reliably predicting its response under loading offers great possibilities for brain injury prevention, disease prediction, and surgical guidance. Such models can provide access to data inaccessible through current medical technology, e.g., local stresses and strains within the tissue. However, the brain is an extremely complex organ and shows high structural and mechanical heterogeneity. Therefore, the identification of material parameters that accurately describe the region-dependent mechanical behavior of human brain tissue is crucial. To this end, we have performed multi-modal mechanical testing on human brain tissue from 19 anatomical regions and have used an inverse parameter identification scheme to identify mechanically distinct regions with corresponding material parameters [1]. In a second step, we have investigated the importance of using region-specific material parameters when modelling the full human brain during two exemplary surgical procedures, an indent to the brain surface occurring during needle insertion [2], and brain retraction using different medical devices [3].

Our results show that accounting for region-dependent properties leads to significant differences in the predicted stress and strain state compared to simulations assuming homogeneous material properties. During brain retraction, tubular retractors result in lower average predicted stresses than traditional spatulas, especially in the subcortical structures and corpus callosum. Additionally, we show that changing the location of retraction can greatly affect the predicted stress results.

Our investigations demonstrate how finite element simulations of neurosurgical techniques can provide valuable insight, e.g., when aiming to minimize trauma during surgical procedures. The identified parameters can contribute to more precise computational models enabling spatially resolved predictions of the stress and strain states in human brains.

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Constitutive modeling of complex materials with machine learning and artificial intelligence
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICS-GUIDED IDENTIFICATION OF DATA-DRIVEN HYPERELASTIC MATERIAL PARAMETERS FROM FULL-FIELD DEFORMATION DATA

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ABSTRACT

Obtaining accurate mathematical descriptors of the nonlinear mechanical behavior of soft heterogeneous materials remains an open challenge in many fields such as biomechanics. While a number of data-driven strain energy functions have been proposed in the last few years, the models have thus far been only applied to learning from homogenized stress and strain data. However, in most realistic scenarios, stress-strain relations vary spatially and material parameters have to be identified from full-field deformations caused by measurable boundary conditions. We develop a physics-guided approach for identifying the parameters of data-driven material models from full-field deformation data. While the method can be readily applied to any data-driven model, we demonstrate its utility via the Neural ODE based model previously proposed by our group [1]. The method relies on minimization of the strong form of the balance of linear momentum. The method is verified by performing finite element simulations with the predicted parameters and comparing to the data collected from the experiments. A number of synthetically-generated and experimental strain fields are used to demonstrate the performance of the proposed method. The method is also compared to existing methods such as the virtual fields method.

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Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELLING THAWING-TRIGGERED LANDSLIDES USING A MULTI-PHYSICS SPH FRAMEWORK

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ABSTRACT

Thawing-triggered slope failures and landslides have become a growing concern in colder regions due to climate change. This has resulted in an increased interest in researching and predicting the behaviour of frozen soils in recent years. However, predicting these phenomena is challenging for computational simulations because they involve complex behaviour of different phases (e.g., soil, water, ice and air), as well as their interactions and phase transformations. Several advanced mathematical models have been developed to tackle these problems, but they are either demonstrated at the constitutive level or incorporated into the standard finite element method (FEM), which is limited to small-deformation problems. On the other hand, rapid mass movements, such as debris flows, caused by thawing permafrost have been reported as typical failure mechanisms. Predicting these phenomena goes beyond the capability of the standard FEM and requires an advanced computational framework that can handle the fully coupled thermal-hydro-mechanical (THM) process, along with the large deformation and flow-failure behaviour of unfrozen soils. This talk discusses the possibility of tackling this challenge using recent advances in multi-physics and multi-phase modelling using the smooth particle hydrodynamics (SPH) method. Frozen soils are considered a tri-phase mixture (i.e., soil, water, and ice), and a robust mathematical framework to describe the fully coupled THM process in this system is derived within the continuum mixture theory and solved using the advanced THM-SPH framework. The proposed computational framework is demonstrated through several numerical verifications and demonstrations, highlighting its usefulness in addressing challenging problems involving thawing-induced large deformation and failures of slope and thawing settlement/consolidation for engineering scale applications.

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Computational and analytical advances in nonlocal modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFICIENT APPROXIMATION OF NONLOCAL ALLEN-CAHN EQUATIONS WITH THE DOUBLE-OBSTACLE POTENTIAL

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ABSTRACT

In this talk, we present an efficient discretization of a nonlocal Allen-Cahn model with the double-obstacle potential.
We propose first and second-order time-stepping schemes with the spectral approximations in space based on a Fourier collocation method. We provide energy stability estimates for the temporal discretization schemes. A particular structure of the model and nonlocal kernel allow for the characterization of the solution in terms of a projection formula. This provides an efficient way to evaluate the solution that avoids solving a nonlinear and nonlocal system. We present several numerical experiments to support our findings.

EQUILIBRIUM THEORY OF BIDENSITY PARTICLE-LADEN SUSPENSIONS IN THIN-FILM FLOW DOWN A SPIRAL SEPARATOR

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ABSTRACT

Spiral gravity separators are devices designed to separate slurry components based on density and size. Previous work explored equilibrium solutions to mixtures of liquids and a single particle species in thin-film flows. Our new analysis extends existing theory to two particle species of different densities. This research unveils a new layer of complexity: particle separation. We expand upon existing theory to understand how particles of different densities segregate within a spiral separator based on its specific configuration. We model gravity-driven bidensity slurries on an inclined spiral by considering particle interactions using empirically obtained formulas for the particle fluxes from previous bidensity studies. In this investigation, we examine a thin-film bidensity particle slurry down a rectangular channel helically wound around a vertical axis. By applying a thin-film approximation, we derive an equilibrium profile for the concentration of each particle species and fluid depth. We identify the influence of design parameters (spiral radius, channel width) on particle concentration profiles in spiral separators. Our work provides an avenue for determining optimal designs for spiral separators across diverse mixtures and flow conditions, revolutionizing particle separation technology.

Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PERIDYNAMIC MICROMECHANICS OF COMPOSITES

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ABSTRACT

Due to the identical operator form of the general integral equation (GIE, forming computational analytical micromechanics, CAM, see 20min video https://lnkd.in/gYp3SJmy) proposed for both local micromechanics (LM, [1], pp. 277-308, 504-510, [3]) and a wide class of nonlocally elastic (strongly weakly nonlocal and strongly nonlocal, [1], pp. 607-794) media, the methods of LM have easily recast into the following peridynamic micromechanics (PM) methods. Nonlinear GIE for LM and PM is obtained [3].

For periodic media, the Discrete Fourier Transform (DFT) is proposed in PM [3] (including the nonlinear problems) as a generalization of LM's counterparts. Many nonlinear phenomena (such as e.g., plasticity, damage, and fatigue) in both the LM ([1], pp. 521-568) and PM are described by energy-based criteria, which, in turn, depend on the second moments of the local fields. Due to the identity of the GIE for LM and PM, the mentioned methods of nonlinear LM are generalized to PM [3].

One proved that Transformation field analysis (TFA) by Dvorak (1992) in LM is a background of clustering discretization method which was generalized to PM [3].

One of the most popular areas of LM is the laminate theory based on the reduction of the equilibrium equation to 1D equation due to the vanishing of the partial derivatives in the transversal directions. Peridynamic counterpart [3] of this vanishing is the integration over the transversal directions. Applications are random and deterministic media, multiphysics, and nonlinear phenomena.

One [2] demonstrated that a body force with compact considered is a very prospective tool for data-driven learning of the surrogate nonlocal constitutive laws of CMs. It gives opportunities to estimate a surrogate nonlocal operator for the field concentrator factors in the phases rather than only an effective operator. Applications are random and periodic media, MD simulations, and machine learning.

CAM (and PM) is presented as a fundamentally new blocked (or modular) structure [3] that is perfectly adapted for the joint development of PM by teams of experts from different scientific areas (e.g. block “peridynamics” and block “micromechanics”). Any knowledge inside one block is not required in another block.

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Modeling and simulation of dynamics, stability and control of aerospace structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STRUCTURAL INFLUENCE OF SHIMS ON METALLIC SINGLE-STRAP JOINT

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ABSTRACT

Aircraft structures are composed of many parts with different shapes, materials, and manufacturing methods. As gaps between parts are unavoidable, shims are often required to fill these apertures. However, shims increase the eccentricity of the joint, intensifying the effects of secondary bending, so they must be considered in structural and fatigue analyses.

Several authors have conducted experimental and numerical studies to understand the influence of shims on the structural behavior of lap joints. There are many other works on the shims on lap joints, but few have addressed the presence of shims in single-strap joints. This work aims to evaluate the influence of solid shims on the stress concentration factor of this type of joint subjected to shear loads.

In this work, 60 configurations of single strap joints submitted to shear loads were analyzed to determine the influence of shims on the stress concentration factor. Three geometrical variables were considered: shim thickness, plate thickness, and fastener diameter D.

The joints were simulated using the finite element software Femap for a linear static solution SOL101. The models were created using hexahedral 8-node solid element CHEXA8 and considering the linear contact BCONTACT method to represent the interface between surfaces. The relative loss of stiffness was presented for every analyzed joint.

The finite element model results showed that an important reduction of joint stiffness can occur when thick shims are used. The stress concentration factors with and without shims, Kt and Kt0, respectively, were obtained. The increase of the stress concentration factor due to the presence of shims was evaluated, resulting in three diagrams that can be used in the aeronautical industry. Diagram #1 presents the Kt/Kt0 for joints with D=4mm, considering several plate and shim thicknesses. Diagram #2 presents the Kt/Kt0 for joints with D=8mm, considering different plate and shim thickness values. For some plate thickness values, the influence of the fastener diameter on the relative stress concentration factor was practically negligible, so Diagram #3 was created. These diagrams and correspondent curves presented a maximum fitting error of 3.4%, showing that they are suitable for primary stages of stress concentration factor predictions.

The use of these diagrams avoids the execution of time-consuming numerical analysis with significant savings for companies that have to deal with shimmed joints frequently, as in the aeronautical industry.

Novel mathematical and numerical models for multiphysics and multiscale systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN INVESTIGATION OF THE FLUID STRUCTURE INTERACTION IN ARTICULAR CARTILAGE ACROSS DISPARATE SCALES

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ABSTRACT

Articular cartilage (AC) is found at opposing surfaces in mammalian joints. It provides a smooth bearing surface, promoting low friction articulation and facilitating continuous operation under relative motion. A lack of cells within AC renders a low capacity for intrinsic healing or repair. This leaves it prone to degeneration and disease, resulting in a high clinical demand for cartilage repair [1]. To streamline treatment, an accurate computational model of the tissue is essential to inform rapid pre-screening of therapeutic interventions. Current models generally use a single-scale approach, which fails to capture the complex multi-scale features of the tissue, including its intrinsic heterogeneity and depth dependant properties [2]. Instead, this project aims to couple an immersed fibrous network (micro-scale) model with a continuum (macro-scale) model, using the Heterogeneous Multi-scale Method [3] to create a multi-scale poroelastic model that can capture the fluid-structure interaction arising within AC across disparate scales. The novelty of the approach lies with using homogenized stress, strain, and velocity from the micro-scale, alongside superposition, to populate the macro-scale elasticity and permeability tensors.

A continuum-continuum model has been developed for validation of the multi-scale poroelastic framework. Currently, a fibrous network representation of the micro-scale behaviour is being integrated into the multi-scale model to include anisotropy and depth dependent properties. Once this continuum-fibre coupling has been established, zonal structuring will be introduced, and the resulting model will be validated against experimental data.

The micro-scale fibre model is based on a regular spring lattice in which lattice bond occupation and spring stiffness can be freely varied, making it an advantageous choice for damage modelling, as fibre anisotropy and damaged tissue can be incorporated by selective modification of the micro-scale elastic elements. Modelling weakening areas of tissue and eventual lesions that arise in damaged cartilage tissue will inform an understanding of the change of behaviour and mechanical properties of the damaged tissue, which could be a critical step to inform clinical interventions for cartilage repair and future replacement.

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Catastrophic failure mechanics and numerical modelling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTATIONAL MODELING OF CUTTING DISC-ROCK INTERACTION IN MIXED GROUND CONDITIONS

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ABSTRACT

In this contribution, we present a simulation tool based on the state-based peridynamic theory, developed to model the interaction between cutting discs of a TBM (Tunnel Boring Machine) and the ground being excavated. As compared to existing TBM performance prediction models, this computational models allows to consider various heterogeneous and mixed ground conditions, different TBM and disc designs, as well as the direct coupling with wear models. Furthermore, the consequences of wear in terms of partially degraded or damaged discs on the excavation performance can be assessed numerically.

The developed model is thoroughly validated using several benchmarks, including indentation tests on sandstone specimens and biaxial strength tests for concrete. The simulation model was further tested by simulating a full-scale LCM (Linear Cutting Machine) test conducted on Colorado Red granite, and the resulting cutting forces at various disc spacings are compared with experimental data.

To investigate excavation in mixed ground conditions, which can lead to abnormal tool wear and even failure, an LCM experiment is performed where the cutting disc excavates through a series of rocks with a high contrast in UCS (Uniaxial Compressive Strength). These experiments successfully identify an overshoot in the cutting force as the disc enters the rock domain with a higher UCS which can cause localized damage to the cutting disc. The cutting forces obtained from scaled-down simulations using the developed model for mixed ground excavation scenarios exhibit qualitative agreement with the aforementioned LCM experiment.

Additionally, the simulation model is equipped with an abrasive wear model, which is verified using analytical solutions. This implemented wear model is able to identify the changes in wear rates as the cutting disc excavates through varying rock formations. Finally, the versatility of the simulation model is demonstrated by investigating various aspects of the cutting disc-ground interaction, including the efficiency of excavation with varying disc geometries.

Advanced discretization schemes and solution strategies for computational structural dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FREE AND FORCED VIBRATIONS OF SHEAR DEFORMABLE CRACKED BEAMS

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ABSTRACT

The presence of concentrated cracks has gained over the years a great deal of attention in view of their strong influence on the vibrational properties of beam structures. The latter influence is due to the local flexural stiffness decay around the damaged cross section that has been widely modelled by making use of the Euler-Bernoulli beam model. Although analogous crack models have been formulated for shear deformable beams, only recently researchers working on the subject focused on convenient formulations of advanced procedures to deal with multiple cracks [1].
Recently, the authors have contributed to the problem by providing an exact distributional model for free vibrations of shear-bending multi-cracked Timoshenko-Ehrenfest beams [2]. The original contribution consists in the adoption of the theory of distribution to treat multi-cracked beams as undamaged beams leading to exact closed form solution of the relevant mode shapes.
The latter achievement is exploited in this work to provide explicit expressions of the so-called Green's functions delivering the forced response in the case of harmonic concentrated loads considering both the undamped and damped vibrations. Spatial convolution of the Green's functions allows the evaluation of the response of multi-cracked beams to distributed loads.
Finally, the proposed exact distributional approach is adopted for assessing the response when the beam is subjected to a generic intensity time history. The latter result is obtained via combination of the Green's functions with the direct and inverse Discrete Fourier Transform (DFT), and allows evaluating the response of shear deformable beams with multiple cracks to arbitrary loading conditions.

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Modeling and inverse design of architected materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

OPTIMIZING STRUCTURES THROUGH GENERATIVE ARTIFICIAL INTELLIGENCE: CASE STUDY ON A CANTILEVER BEAM MADE OF DIFFERENT MATERIALS

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ABSTRACT

Conventional topological optimization techniques focus on deriving optimal structures through a predefined set of constraints and objectives, often limiting the modifications to changes to already existing designs. Notably, these methods operate within the constraints of a known material composition, restricting the ability to alter materials. Another traditional constraint lies in the inability to generate structures from scratch, necessitating initial designs for subsequent reduction to achieve specific performance goals. To overcome these limitations, novel approaches involving machine learning, specifically deep learning techniques, have been proposed in the literature. However, state-of-the-art solutions have not been adopted yet in the field of structural mechanics. In this context, this work aims to develop a generative artificial intelligence-based framework for an enhanced topological optimization of structures. Variational autoencoder were considered to the purpose. Such algorithms learn from diverse structures and subsequently generate optimized designs. This expands the optimization scope to generating structures from scratch and allows including multiple objectives, such as maximum stress, weight reduction, vibration modes, or mechanical wave propagation. The framework's transformative impact on topological optimization was exemplified through a specific case study involving a fixed end beam. The model was trained over a numerical dataset including the response of structures made of different materials, developing the capability to generate optimal designs for a fixed end beam configuration. This innovative approach not only broadens the scope of topological optimization, but also showcases its adaptability to specific structural configurations, offering promising prospects for a more comprehensive and versatile structural design process.

Numerical modelling of composite materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL STUDY OF FORCED VIBRATIONS OF FLAX-EPOXY COMPOSITE STRUCTURES WITH A PERTURBATION METHOD.

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ABSTRACT

This study deals with response curves computations for forced vibration of composite structures made of a flax fiber-reinforced epoxy matrix. This kind of bio-based composites has the advantage to present greater damping compared to synthetic fibers. Moreover, this damping is frequency-dependent[1], meaning that it is different for each vibration mode. So, one have to consider a viscoelastic law to describe this property in the case of bio-based composites. In this study, two different constitutive equations are considered : the generalized Maxwell model and the fractional derivative Zener model[2]. As these laws are nonlinear in frequency, this leads to a nonlinear forced vibration problem. To solve this problem, the asymptotic numerical method [3] is used. It combines a perturbation technique and a finite element method. The nonlinear initial problem is transformed into a succession of linear ones that admit the same tangent matrix and different right-hand sides. This permits to reduce the computational costs compared to classical iterative methods. Numerical results obtained with this approach are compared, in terms of damping frequencies and structural loss factors, to those obtained when considering the free vibration case.

Data-driven approaches for solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE QUEST TO FIND THE ANALYTICAL SOLUTION OF COOK'S MEMBRANE WITH NEURAL NETWORKS

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ABSTRACT

Cook's membrane has been a popular boundary value problem used to benchmark performance of incompressible elasticity. Despite its popularity, the analytical solution of this linear elasticity problem is not known and hence Richardson's extrapolation is often used to check convergence. This talk presents a technique that uses multiple neural networks to generate basis functions to span the solution space. By mapping the irregular domain onto a square, we introduce a technique where a finite element solution is first used to provide the useful inductive bias to generate the appropriate basis that generates an accurate approximate solution. Following this step, a genetic algorithm is then used to convert the neural network learnt basis function into the analytical form, thereby enabling the analytical solution to be expressed as a polynomial in a feature space. This generalized version of the neural additive method [1][2] is crucial to overcome the curse of high-dimensionality of the symbolic regression problem in multi-dimensional settings. While the heuristic nature of the search does not yield the exact solution for Cook's membrane, we find a few close approximations of the solutions that yield 0.01% collocation errors. The analytical solutions expressed in both Airy stress function and as displacement field are compared.

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Fluid dynamics and SciML: Navigating challenges and seizing opportunities
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICS-INFORMED DATA-DRIVEN RANS FRAMEWORK FOR WALL-BOUNDED FLOWS: A PRIORI AND A POSTERIORI VALIDATION

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ABSTRACT

Numerous Tensor Basis Neural Network (TBNN) frameworks [1] have recently emerged in the literature as data-driven constitutive models, embedding inherent physical invariance properties to augment turbulence Reynolds-Averaged Navier-Stokes (RANS) modeling. Despite their proven success, persistent uncertainties surround the choice of the integrity tensor basis [2], coupled with a notable lack of attention and transparency in data analysis and training strategies. This paper aims to rectify and tailor TBNN through a comprehensive application to two distinct wall-bounded flows of increasing complexity: Plane Channel Flow (PCF) and Square Duct Flow (SDF).

In the present work, thorough analyses on the integrity tensor basis and the raw training data are conducted for each flow case to establish optimal and physically sound tensor basis models. Subsequently, augmented TBNNs based on this modeling are trained using state-of-the-art strategies to achieve a balanced prediction of the full Reynolds stress anisotropy tensor (RST). A priori results obtained by the proposed framework are in very good agreement with the reference data from Direct Numerical Simulations (DNS) in both interpolation and extrapolation scenarios [3]. When the learning becomes more challenging, we suggest some numerical strategies (e.g. based on Transfer Learning (TL) in order to leverage our prior knowledge and mitigate this problem.

A challenge might arise when incorporating data-driven RST closures into RANS equations, as maintaining model consistency becomes crucial. This concern, particularly evident in potential inaccuracies related to the mean velocity profile, is addressed in our approach. The proposed neural network models are seamlessly integrated into a customized, in-house RANS solver for a posteriori validations, employing an iterative substitution framework. A comprehensive set of case studies is meticulously examined by introducing TBNN contributions in varying components of the RANS solver to scrutinize error propagation. Initial findings at this stage provide valuable insights, positioning the proposed approach as a competitive alternative to traditional RANS models.

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Causal discovery and graphical causal models
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A CAUSALITY-DEEPONET FOR CAUSAL RESPONSES OF LINEAR DYNAMICAL SYSTEMS

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ABSTRACT

In this talk, we will present a DeepONet structure with causality to represent causal linear operators between Banach spaces of time-dependent signals. The theorem of universal approximations to nonlinear operators is extended to operators with causalities, and the proposed Causality-DeepONet implements the physical causality in its framework. The Causality-DeepONet considers causality (the state of the system at the current time is not affected by that of the future, but only by its current state and past history) and uses a convolutiontype weight in its design. To demonstrate its effectiveness in handling the causal response of a physical system, the Causality-DeepONet is applied to learn the operator representing the response of a building due to earthquake ground accelerations. Extensive numerical tests and comparisons with some existing variants of DeepONet are carried out, and the Causality-DeepONet clearly shows its unique capability to learn the retarded dynamic responses of the seismic response operator with good accuracy.

Multi-scale and machine learning-based modeling methods for optimization and design of composites
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INVESTIGATION OF OFF-AXIS TENSION FAILURE MECHANISMS IN TRIAXIAL BRAIDED COMPOSITES THROUGH MESOSCALE SIMULATION

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ABSTRACT

The intricate braided architecture makes the two-dimensional triaxial braided composites (2DTBC) exhibit distinct local stress states under uniaxial tensile load and also causes their failure mechanisms to be complex and dependent on the loading angle [1-2]. This study develops a full-scale mesoscale finite element model matched to experimental specimens to investigate the mechanical response and damage characteristics of the 2DTBC under off-axis tensile loadings. The numerical simulation successfully predicts the mechanical performance across five off-axis angles: 0°, 30°, 45°, 60°, and 90°. By capturing the diverse loading responses, the model reveals the transformation of failure behaviors and damage morphologies as the loading angle varies. The results demonstrate that when the external load is applied in alignment with the fiber bundle direction of the specimen, the primary failure mechanism involves the fracture of the load-bearing fiber bundles. Conversely, when the loading direction forms an angle with any of the fiber bundles, the failure mechanism shifts to local shearing of bias fiber tows. Furthermore, both the numerical results and experimental observations emphasize the substantial impact of the free-edge effect [3], which causes premature failure of the specimen on the off-axis tensile loading. In addition, the discussion of the Hashin shear factor further clarifies the mechanism of the influence of shear stress on the failure behavior under different off-axis loadings. This study provides valuable engineering insights for optimizing the performance of 2DTBC in advanced applications.
Keywords: Triaxial braided composites; mesoscale finite element model; off-axis tensile; free-edge effect;

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Machine learning and multiscale modeling for complex materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFICIENT GRAPH NEURAL NETWORKS FOR STRUCTURAL ANALYSIS OF STIFFENED PANELS

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ABSTRACT

Machine learning (ML) and deep learning (DL) techniques have gained significant attention as reduced order models (ROMs) to computationally expensive structural analysis methods, such as finite element analysis (FEA). Graph neural network (GNN) is a particular type of neural network which processes data that can be represented as graphs. This allows for efficient representation of complex geometries that can change during the conceptual design of a structure or a product. In this study, to address such computational challenges in structural analysis, we propose a novel graph embedding for the efficient representation of 3D stiffened panels by considering separate plate domains as vertices. This approach not only simplifies the representation of complex geometries but also adapts to changes during the design phase. Employing Graph Sampling and Aggregation (GraphSAGE), our model predicts stress distributions in stiffened panels under varying geometrical configurations, material properties, and loading conditions.

One feature of our research is the comparative analysis against traditional finite element-vertex graph representation. This comparison showcases the computational efficiency of our GNN-based model, particularly in saving GPU memory and GNN training time. In addition, a comprehensive parametric study is performed to examine the effect of structural variables on stress predictions. A wide range of geometries is considered, including material nonlinearity, a few boundary conditions, together with uniform and patch loading at various positions. Our results reveal the GNN model's remarkable efficiency in predicting stress distributions, often surpassing the performance of traditional methods in complex scenarios. These results not only demonstrate the potential of GNNs as a robust, reduced-order modeling tool for structural analysis but also pave the way for their application in the early stages of structural design.

Modeling and simulation of dynamics, stability and control of aerospace structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VIBRATION CONTROL AND ANALYSIS OF CABLE-DRIVEN DEPLOYABLE TRUSS STRUCTURE MAST

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ABSTRACT

In recent years, due to the gradual complex trend of space missions, the space structures have gradually developed in the direction of large scale and flexibility. Space deployable masts are often used as supporting structures for working platforms of spacecrafts due to their light weight and high expansion-to-retract ratio. However, spacecrafts are often affected by external factors such as space gravity gradient, temperature variation and solar light pressure in space environment. In addition, during active working process such as position and attitude changes or space operations, low-frequency vibration of the extended truss structure is easy to be caused, which decays very slowly in space environment with low damping. If the vibration energy is not controlled, it may adversely affect the entire system. Therefore, implementing an appropriate vibration control is crucial for ensuring the deployable mast's operation. This study specifically focuses on a deployable truss structure mast that employs cables as actuators. The research includes the optimization of actuator positions and the design of control laws, taking into account both unilateral and saturated constraints of the cable actuators. First, modal information about the structure is obtained using the commercial software ANSYS. And the model of the truss structure is established with the second Lagrange equation based on finite-element-method. Second, the criteria of position optimization of actuators and sensors is constructed using Gramian matrices that can describe the controllability and observability of the control system. The actuator position optimization method is devised by the controllability principles and the genetic algorithm. Finally, a deployable truss structure mast consisting of four units is simulated and analyzed. The results demonstrate that the proposed actuator optimization position and the control law effectively mitigate the vibration and ensure the stable operation of the deployable mast.

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SENSING VEHICLE DESIGN OPTIMIZATION FOR BRIDGE INDIRECT STRUCTURAL HEALTH MONITORING BASED ON SURROGATE MODEL

Andres Felipe Calderon Hurtado[*1], Mehrisadat Makki Alamdari[1], Elena Atroshchenko[1], Chul-Woo Kim[2] and Kai Chun Cahng[2]*

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ABSTRACT

Bridge indirect structural health monitoring (BISHM) using drive-by bridge inspection has been widely studied over the last decade. Such methodologies consist of assessing bridge damage from the coupled bridge-vehicle response measured by an instrumented vehicle. Certainly, most studies consider commercial vehicles as sensors, which limits the applicability of this technology since the damage assessment performance depends on the sensing vehicle characteristics. Looking forward to a future in which autonomous vehicles are designed and used specifically for bridge inspection, this work presents a sensing vehicle design optimization to maximize the damage assessment performance using drive-by inspection in a numerical case study. First, a methodology based on the analysis of the frequency domain representation of the signal recorded by the vehicle is presented to identify bridge damage at different locations. The output of the framework corresponds to two probability distributions, one for healthy samples and one for damaged samples, respectively. The distance between these distributions is used as the objective function of optimizing the vehicle properties. Then, a Kriging meta-model of the distance between probability distributions is constructed from the results obtained from multiple vehicle configurations. Such a model is then used to perform the optimization of the vehicle characteristics that maximize the distance between the healthy and damaged samples' distributions. Finally, vehicle design guidelines are presented in terms of non-dimensional parameters that relate to the vehicle and bridge properties.

QUANTIFYING UNCERTAINTIES IN MODELING CHOICES FOR TIME-SENSITIVE APPLICATIONS

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ABSTRACT

“Quantifying uncertainties in modeling choices for time-sensitive applications”
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Multiphysics simulations involve a number of modeling choices, including material strength, meshing strategies, and equation of state. These methods are often verified using ideal scenarios (e.g., uniform mesh, analytic solutions available), but there are scenarios during which this approach is not feasible. Planetary defense, a research subject focused on protecting Earth from impacts from potentially hazardous objects (PHOs), is a matter of both national and global security. Simulations of planetary defense applications involve spatial scales of hundreds of kilometers and temporal scales on the order of seconds or longer. Thus, modeling choices must be made to ensure that knowledge can be obtained in a timely manner, as mission design can take years and flight time from Earth to a PHO can take from 6 months up to years. Understanding how these choices (e.g., a varied mesh resolution that is more resolved around the impact point and less resolved at the edges) contribute to overall uncertainty is of utmost importance in preparation for a variety of potentially catastrophic scenarios. In this work, we examine how specific modeling choices contribute to uncertainties in numerical simulations as a means of better understanding how to best interpret results and apply the appropriate error bars given a time-sensitive scenario, such as an impending meteor strike. We also discuss the simulations run as part of the Near Earth Object Table Top Exercise of 2024, which considered a number of possible mitigation strategies and associated timelines.

Multiscale modeling of dynamics in complex media and metamaterials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TRANSIENT NONLINEAR RESPONSE OF RESONANT METAMATERIAL ARRAYS UNDER IMPACT LOADING

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ABSTRACT

Metamaterials (MM) can be designed to attenuate the energy transfer induced by impact and blast loadings. These materials employ local resonance with resonators tuned for a range of frequencies for stress wave mitigation. Even though traditional Frequency Domain (FD) methods are commonly used to analyze the idealized conditions, understanding the time domain response is crucial for more realistic results the transient response of wave propagation in periodic media can more naturally be modeled in Time Domain (TD). Moreover, TD analysis is necessary when nonlinear processes such as fracture are considered. This work analyzes the time domain response of a low-frequency resonant ceramic MM under impact loading using the Johnson-Holmquist II (JH-2) material model. The performance of the MM is compared to monolithic slabs and other microstructured designs in terms of stress wave mitigation, peak load retardation, and energy transfer. The simulations are conducted with different boundary conditions and domain sizes. Loading is applied as plate impact and point impact for two different MM designs. Results show that the MM performed better in delaying and reducing the peak energy transfer than the other designs. Additionally, we found that the wave anisotropy of the metamaterial design further improved its performance in terms of stress wave mitigation. The unique directional properties of the metamaterial sample allowed for more efficient energy transfer, resulting in overall enhanced performance compared to the other designs. The study concluded that resonant ceramic metamaterials are a promising new class of materials with unique and tunable properties that can be used for protective and structural applications.

Next-generation numerical methods for coupled multiphysics problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ANALYSIS OF A MIXED FEM WITH EXACTLY DIVERGENCE-FREE MAGNETIC FIELD FOR THE STATIONARY MHD PROBLEM

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ABSTRACT

In this work we analyze a mixed finite element method for the stationary incompressible magneto-hydrodynamics problem providing an exactly divergence-free approximation of the magnetic field. The method is based on the introduction of the volume current density as a further unknown leading to a mixed formulation where the primary magnetic variables consist of the volume current density, the magnetic field, and a Lagrange multiplier included to enforce the divergence-free constraint of a magnetic field, whereas the hydrodynamic unknowns are the velocity and pressure. Then the associated Galerkin scheme can be defined by employing Nédélec and Raviart-Thomas elements of lowest order for the volume current density and magnetic field, respectively, discontinuous piecewise constants for the Lagrange multiplier and any inf-sup stable pair of elements for the velocity and pressure, such as the Mini-element. The analysis of the continuous and discrete problems are carried out by means of the Banach-Nečas-Babuška theorem and the Banach fixed-point theorem, under a sufficiently small data assumption and quasi-uniformity of the mesh, the latter for the discrete scheme. Finally, we derive the corresponding Cea's estimate and provide the theoretical rate of convergence.

THEORETICAL DEVELOPMENTS ON A KINEMATICALLY-EXACT ROD MODEL FOR THIN-WALLED MEMBERS WITH CROSS-SECTIONAL DEFORMATION AND FINITE STRAINS

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ABSTRACT

This work presents theoretical developments on a kinematically-exact rod model to incorporate cross-sectional deformation (warping and distortion) degrees of freedom for thin-walled members, with associated shell bending effects of the walls and a polyconvex constitutive equation for finite strains. The model´s weak form and associated tangent operator are derived, aiming for future numerical implementation through the finite element method (this is currently under development and will be addressed in a subsequent work; some preliminary results may be shown). We believe the model is useful for developing a robust framework for the simulation of frame structures consisted of thin-walled members, in which local effects (e.g. web and flange local bending and buckling) are prone to arise and stand as typical design constraints in most design standards worldwide. The model´s displacement field allow for the traditional cross-sectional rigid body motion, along with the walls´ mid-line in- and out-of-plane deformations (first-order in-plane distortion and out-of-plane warping, respectively, herein called primary deformations) and a kinematically-exact rotation for the walls´ out-of-mid-line points (herein called secondary deformation). The rigid body motion is parametrized as usual for geometrically-exact beams, whilst primary deformations are described by linear combinations of distortion modes, borrowed from the so-called Generalized Beam Theory (GBT). The (shell-like) rotation that defines the secondary deformation is described as a function of the walls´ mid-line displacement field and is parametrized using Kirchhoff-Love shell assumptions. The use of a polyconvex hyperelastic constitutive equation guarantees material stability for the solution at finite strains situations. Although rod models with cross-sectional deformation may be found in the literature (see, e.g., Gonçalves, Rito-Côrrea and Camotim [1]), they invariably neglect higher order strain and/or constitutive terms, which may be relevant to capture some usual global buckling modes, as shown in [2]. Enabling these higher order deformations with local effects is the novelty of this work.

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Scientific machine learning for geophysical applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PROBOOST: PROBABILISTIC BOOSTING FOR FORECASTING RARE AND EXTREME EVENTS. CASE STUDIES IN SPACE WEATHER PREDICTION

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ABSTRACT

In the field of space weather, we are interested in forecasting rare and extreme events, while most of the time the output of interest is in quiet-time condition. Hence, the typical space weather dataset is highly imbalanced with the interesting events being very rare. In such a scenario typical machine learning (ML) regression methods fail to perform well on the events of interest. Moreover, in order to be actionable any forecast needs to come with a estimate of its uncertainty. Once again, typical ML methods for regression output a single scalar value, with no indication of confidence intervals.

In this work we present ProBoost (Probabilistic Boosting), which is inspired by the popular Gradient boosting method and whose aim is to simultaneously: 1) boost the performance of weak learners, especially in the presence of rare events; 2) provide a reliable uncertainty estimate of the predictions.

The engine under the hood of ProBoost is ACCRUE (Accurate an Reliable Uncertainty Estimate), an a-posteriori, model agnostic method for uncertainty quantification, which will be introduced (Camporeale, E., & Carè, A. (2021). Accrue: Accurate and reliable uncertainty estimate in deterministic models. International Journal for Uncertainty Quantification, 11(4).)

Finally, we will present examples of applications of ProBoost in the context of real-time space weather predictions, developed and operationalized by the Deep Learning Laboratory at the University of Colorado, Boulder, and freely available to the general public (https://swx-trec.com/)

Mesh-free particle methods for multi-physics problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SPH CONTINUUM-BASED MODELLING OF FLUVIAL ICE DYNAMICS

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ABSTRACT

Numerical modelling of river ice dynamic processes, such as ice jams along large river extensions can help to better understand and predict these natural incidents and their impacts. However, the numerical methods, associate to these simulations, demand the ability to process vast amount of data at large spatial scales. The smoothed particle hydrodynamics (SPH) method offers the ability to deal with the highly dynamic ice-water interaction due to its lagrangian nature at reasonable computational cost. For such reason, in this work, we proposed a two-phase fully Lagrangian continuum-based SPH numerical method to simulate river ice dynamics. The method solves the depth-averaged Navier- Stokes equations, also known as the shallow water equations (SWE), for both water and continuum. A SWE solver offers a greater computational affordability for large scale simulation with a dominant horizontal dimension. The computation domain is represented by a set of particles that are used to represent a fixed-volume column of material. The riverbed is defined as a set of fixed particles that are coupled to the fluid particles in a well-balanced scheme that allows to simulate riverbed slopes properly by using a variational approach and a bed filter [1]. Likewise, ice is modelled with SPH, where each particle is defined as column of ice volume that interacts with fluid particles by applying ice driving forces. These forces include the water drag, the riverbank contact and the gravity as external forces, and the ice resistance as an internal force. This internal force is adopted from a viscous-plastic constitutive law, allowing to simulate ice accumulation processes such as those in the presence of ice jams [2]. As part of the results, the proposed method was validated with different 1D and 2D benchmark cases. The agreement between the mathematical formulation and the motion evolution of ice in the river is of primary importance to the purpose of this work. Factors like bed friction, wind force, ice-growth and de-icing also influence the dynamics of ice and fluid, and these can be included in further work using this simulation as a base model.
Keywords: ice jam, river ice, SPH method, shallow water equations, ice-fluid coupling model. References:
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Modeling and simulation of coupled processes in geological media
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THREE-FIELD MODEL FOR WAVE PROPAGATION IN POROUS MEDIA BASED ON MIXTURE THEORIES

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ABSTRACT

Simulations of wave propagation in porous media are important to the understanding of various phenomena, such as seismic effects and non-destructive testing. The derivation and implementation of finite element analysis for a fully dynamic three-field deformable porous media model based on the de la Cruz and Spanos (dCS) theory [1] is presented. The dCS theory accounts for the fluid viscous dissipation mechanism and nonreciprocal solid-fluid interactions, which are neglected in Biot theory [2]. While the Biot theory is based on experimental data, the dCS theory is derived from mixture theories associated with the volume fraction concept and representing the connection between micro and macro pore scales. dCS results presented build upon recent FE model for quasi-static analysis [3]. Here, for the fully dynamic case incorporating both fluid and solid inertia, the accuracy and robustness of the FEA model is verified by wave propagation examples in one and two dimensions. Time integration scheme utilized and the changes in convergence rates according to how strongly coupled is the system will be discussed. The required element approximation order for all variables to ensure numerical stability will be demonstrated. The presented model is compared with the results from Biot theory, allowing one to observe the differences between the two theories and their relevance. The solutions in the time and frequency domain are also discussed, where the analysis of the correspondent eigenproblem leads to important information regarding wave velocity and attenuation.

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Recent advances in numerical methods for interface problems
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MULTILAYERED POROELASTIC MEDIA INTERACTING WITH FREE FLUIDS

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ABSTRACT

We will discuss some recent results on the well-posedness of a nonlinear fluid-structure interaction problem involving multi-layered poroelastic media interacting with the flow of a viscous, incompressible fluid.

THE SPECTRAL ELEMENT METHOD FOR THE VIBRATIONS OF CRACKED FRAMES

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ABSTRACT

The presence of damage or impairments in frames can strongly influence its dynamic properties and, subsequently, its response when subjected to external loads. For the evaluation of the dynamic response of structures, approximate solutions based on the Finite Element (FE) models are usually employed, considering additional nodes at the cracked sections. Within this framework, assemblage of stiffness and mass matrices is required based on the static shape functions of the elements. Subsequently, an eigenvalue problem has to be solved to infer the eigenproperties of the structure; in addition, when external loadings are applied, direct integration or modal superimposition are usually employed to assess the response. Alternatively, a continuous approach can be adopted to get rid of the approximations of the FE strategy. More precisely, a continuous strategy, namely Dynamic Stiffness Method (DSM), requires the assemblage of a frequency dependent dynamic stiffness matrix, whose zeros represent the eigenfrequencies of the structure [1]. Within this context, the forced vibrations are usually treated with the so-called Spectral Element Method (SEM), which employs the dynamic stiffness matrix and frequency dependent shape functions.
This study, based on a closed-form solution proposed for Timoshenko beams with multiple cracks [2], extends the SEM to the case of cracked structures. The mentioned exact distributional approach is adopted to formulate an exact explicit expression of the frequency dependent dynamic stiffness matrix accounting for multiple concentrated cracks. The closed form expression of the DSM allows the assemblage of the global DSM of a structure to conduct the free vibration analysis of damaged framed structures. This approach has the advantage to avoid any numerical procedure for the construction of the DSM as well as the introduction of further degrees of freedom in correspondence of the damaged sections, keeping the size of the problem the same as in the intact configuration. Frequency dependent shape functions are subsequently inferred, thus allowing the evaluation of the nodal forces and the application of the SEM to cracked structures without adding degrees of freedom at the discontinuous sections.

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Computational design of mechanical metamaterials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE MODELLING OF SHOCK ABSORBING HYPER-ELASTIC METAMATERIALS

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ABSTRACT

Metamaterials are artificial designed materials that exhibit apparent exotic properties at the macroscopic scale which are presently a topic of large interest in material science. The goal of this work is the development of computational tools for designing a specific branch of metamaterials: shock-absorbing dissipative metamaterials, aiming at two goals. The fast (macroscopic) shape recovery after impact from an external impactor and the subsequent loading release. This is a very appealing property to absorb high-frequency impacts: the absorbing device readily recovers, immediately after any impact, its original shape and its energy-absorbing capacity becoming available to absorb the next mass impact.

Standard hyper-elastic materials fulfil the non-dissipation paradigm, but, if this paradigm is broken, they may exhibit relevant mechanical dissipation as the free energy turns non-convex. This work focuses on these cases at the macroscopic scale, yielding shock-absorbing metamaterials exhibiting dissipative behaviour at the upper scale, but made of polyconvex hyper-elastic materials at the low scale. The coupling between both scales is, then, responsible for the exotic dissipative behaviour at the macroscale.

In this work, a microscale made of a buckling lattice of periodic cells is conceived as a mechanism to achieve the non-convexity of the free energy at the macro-scale, where some of their elastic members exhibit an appropriated buckling behaviour. The structural behaviour of the slender buckling members in the lattice (typically beams) is described in terms of degenerated kinematics, and, in turn, the upper scale is naturally described using standard 2D/3D solid formulations. The problem of translating the standard multi-scale formulations, established for settings in which the macro-scale and the micro-scale domains are described in a unique dimension space, into the intended unmatched dimensions case is solved by introducing an Ersatz material into the formulation. The lattice is designed as a sequence of sufficiently dimension-perturbed buckling layers so that instabilities arisen when the RVE is constituted by a number of a homogeneous set of layers is precluded. As for the structural modelling of the buckling-beam members in the microscale lattice, the elastic large strain Timoshenko-like beam combined with a least energy bifurcation criterion is considered. in order to represent the microstructure.

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ENERGY ABSORPTION DESIGN AND WORKING MECHANISM FOR SOLID/LIQUID HYBRID COMPOSITE

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ABSTRACT

Besides conventional solid-based energy absorption/damping materials, the solid-liquid hybrid system potential applications in mitigating impact/blast loadings. It was reported that a solid-liquid hybrid system including water and hydrophobic nanoporous materials shown an energy absorption/damping ability. The energy absorption process is performed through liquid phase transformation induced by the applied pressure: from the original macro-phase (with a low potential state) to the nano-phase with a high potential state (the liquid inside nonwettable nanopores). In addition, the reverse phase transformation process might be possible after unloading, suggesting that the hybrid system can be fully recovered after unloading. The above energy absorption procedure closely depends on (1) the wetting behavior of nanopore; (2) the infiltration behavior of nanopore; (3) the transport behavior of liquid inside nanopore. Based on computational simulations, the above important scientific issues can be clarified, and the energy absorption/damping mechanism as well as the influence factors of the system energy absorption density are further identified. The present study will provide an important help on designing new energy absorption materials, and can also boost the development of the multiscale theory associated with mechanics in multi-disciplinary areas.

Modeling, simulation, and AI for ultrasonic NDT and SHM
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ZERO-GROUP-VELOCITY LAMB WAVES GENERATED AND DETECTED BY PIEZOELECTRIC DIRECT-WRITE TRANSDUCERS FOR CONTINUOUS MONITORING OF FASTENER TIGHTNESS

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ABSTRACT

Continuous monitoring of the tightness status of a fastener structure is of paramount importance in many industries, as a slight loosening may pose a significant threat to the integrity of structure. In this paper, we propose using Zero-Group-Velocity (ZGV) Lamb waves generated and detected by in-situ piezoelectric Direct-Write transducers (DWTs) to monitor fastener loosening status and evaluate stress distribution around fastener holes. Unlike the conventional bulk wave method, the ZGV Lamb wave based method with confined energy could effectively reveal the stress level near the fastener hole at low frequency. Usually, the ZGV Lamb wave is excited and detected by non-contact laser ultrasonic techniques, which may have a few issues for real-time inspection. With features of high conformability, low cost, low profile, etc., the piezoelectric DWTs are directly printed on the fastener structure to generate and detect ZGV Lamb waves for real-time inspection. To demonstrate the proposed method, the suitability of DWTs to generate and detect ZGV Lamb waves is first discussed. Next, the dispersion relation of a fastener plate structure is investigated with various preloading force. Acoustoelastic effects from out-of-plane stresses are considered in this study. A circular array of DWTs is then printed around the fastener hole and the loosening status of the fastener is determined by examining the frequency shift of the ZGV Lamb Wave. This circular array reflects stress levels near the hole region, which overcomes the disturbances caused by multi-mode conversions and wave scattering. The developed method has great potential applications in providing very reliable and accurate continuous monitoring of the tightness of fastener structures.

Recent advances in discretization techniques for coupled problems in incompressible fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL METHODS FOR IMMISCIBLE INCOMPRESSIBLE MULTIPHASE FLOWS WITH THERMAL CONVECTION.

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ABSTRACT

We present a numerical approximation method for immiscible incompressible multiphase flows problems with thermal convection. The fluids properties (e.g. density, viscosity, thermal conductivity) vary in space and time and are assumed to be dependent of the density, thus the resulting problems are governed by a mass conservation equation, the incompressible Navier-Stokes equations and the temperature equation. The formulation uses the density, pressure, momentum and internal energy as primary unknowns which allows us to introduce a scheme with time-independent stiffness matrices. The spatial discretization is based on continuous finite element methods. Stability and space-time errors estimates will be discussed before we present numerical investigations with manufactured solutions and setups with turbulent thermal convection.

Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELLING OF SOIL-ROOT INTERACTIONS IN GEOMECHANICS WITH THE G-PFEM

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ABSTRACT

Most engineering techniques used to stabilise slopes are very carbon intensive: concrete piles, gabions, crushed rock, geogrids or meshes, steel anchors and shotcrete, etc. Moreover, climate change is believed to have an adverse effect on the stability of slopes due to the degradation of the soil strength and the increase of water pressure. Therefore, the use of carbon-intensive techniques does not seem consistent with the current greenhouse gas emission targets.

The use of green engineering techniques, such as the use of plants to stabilise slopes, can be a clean and sustainable solution to this problem. The use of plants has a direct benefit in stopping deforestation, sustainable land use and restoring nature.

The current state of the art for characterising the mechanical effects of plant roots in soils is limited. This has direct implications for the application of vegetation in slope stability.

Numerical analysis of this problem can bring light into the darkness. The analysis of soil-root interactions requires advanced techniques: modelling the hydromechanical properties of rooted soils coupled with the mechanical strength contribution of the roots. Furthermore, a large-deformations framework is needed to validate the results with experiments (modelling of plant extraction or landslides).

Our contribution in this area is the development of the Geotechnical Particle Finite Element Method (G-PFEM) for modelling soil-root interactions. Different modelling approaches are investigated for the modelling of structural roots and the constitutive behaviour of the soil and the rooted soil. Simulation results are compared with interaction tests and slope stability models are presented.

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Numerical modelling of composite materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

QUALIFICATION OF A PRM CONNECTION FROM ASSEMBLED I-BEAM TO ASSEMBLED COMPOSITE TUBULAR COLUMN WITH FILLET WELDS

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ABSTRACT

The high level of implementation in steel structures in the infrastructure field, has led that the industry and academic institutions do research on the topic. This, with the aim of creating reliable and feasible methodologies in factories devoted to the construction area.
A crucial aspect of steel structures has been the design and manufacture of connections as they have a great participation in the response of dynamic and static loads. The type of connection which requires to be researched in depth are rigid connections. In other words, these can provide lateral stability in structures against seismic forces. For this reason, the current investigation emphasizes on these group of connections. Similarly, connections are studied to be resistant and functional, which can guarantee a satisfactory behavior to endure seismic loads. Also, it is necessary to evaluate manufacturing methodologies that are cheap and easy to apply. Weld in connection is a fundamental aspect for its construction, and it is one of the most expensive components in the whole connection due to the material preparation and rigorous quality controls.
The main purpose of this research is to assure that a composed tubular column type connection throughout fillet welding processes connected to a I beam shape with fillet weld too, present a structure stability; this is achieved through a connection qualification where it is exposed to a cyclic load controlled in a lab. It is expected that the dynamic response has an acceptable behavior established in the specifications of the American Institute of Steel Construction AISC chapter AISC-348 about seismic provisions.

Although similar connections have been pre-qualified, these have presented some difficulties to the industries since the weld allowed in these connections is a complete penetration weld which requires the material preparation by bevels; additionally, tests are more rigorous resulting in more expensive processes for its construction. Therefore, this research aims analyzing the dynamic structural response of connections where fillet weld is used to build columns and beams.

During the qualification process, it is determined to evaluate the connection dynamic behavior and the generation of the plastic articulation as an energy dissipation mechanism. Due to this, it is recommended to make the comparison between the lab results and the finite element numerical modeling.

Emerging topology and shape optimization techniques in computational design of materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

POLYCRYSTALLINE MATERIAL DESIGN: A DATA-DRIVEN APPROACH WITH BAYESIAN OPTIMISATION

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ABSTRACT

Over the past decades, the modelling of complex material systems has been widely explored, which has led to accurate and efficient representations of the constitutive response of materials employed in the automotive, aeronautical and aerospatial industries. Coupled with this advent, the rapidly growing computational power available allows running an increasing number of simulations at a fast pace, which is required to match industrial needs. The combination of these topics leveraged the application of the so-called inverse problems, where numerical tools are used to find solutions for real-world optimisation problems, such as parameter identification, topological optimisation and material design.

In this work, we explore a data-driven framework for the design of polycrystalline materials, inspired by [1]. Microstructural properties such as phase volume fractions and grain orientation and distribution are analysed, and crystal plasticity models [2] are used to derive the macro- and micro-scale response of the material. For ease of generalisation with available solvers, the task is formulated as a gradient-free optimisation problem, where Gaussian Process regression and Bayesian optimisation are used as the pillars for its numerical solution. The framework allows for the optimisation under uncertainty and its quantification throughout. This strategy efficiently explores the design space and outperforms classical space-filling design of experiments (DoE) strategies, leading to faster optimisations with fewer function evaluations. An in-house tool for the optimisation of numerical responses is used for solving the inverse problem. Finally, given the recent breakthroughs in the solution of the parameter identification problem using composite Bayesian optimisation strategies, as shown in [3], a similar approach is also explored for the material design problem to improve the quality of the used surrogate models.

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Data-driven device and circuits models
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ACCELERATING CODESIGN IN EMERGING COMPUTING

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ABSTRACT

Emerging beyond Von Neumann computing paradigms such as neuromorphic computing and probabilistic computing are gaining traction as conventional systems approach performance saturation. Neuromorphic computing takes inspiration from the organizing principles of the brain (e.g. co-location of memory and compute elements, massively parallel computation, online learning, etc.) to efficiently exploit the physics of computation in hardware. Probabilistic computing is another emerging field that can benefit from the inherent stochasticity found in neuromorphic systems and these approaches can be complimentary. Typically, solutions in both these fields can span digital, analog, mixed-signal, and emerging beyond-CMOS devices. However, diverse approaches pose significant codesign challenges across the full design stack. For effective collaboration and codesign, we need abstracted device and circuit models that can be co-optimized keeping both hardware, algorithm, and system constraints in mind.

In this talk, I will present two exemplars in multilevel codesign in neuromorphic, and probabilistic computing. I will illustrate how device and circuit abstractions enable faster computation and can be scaled easily for further design space exploration. I will also introduce AI-guided methods to accelerate discovery and codesign.

Our neuromorphic exemplar is a dendrite simulation model based on an analog dendrite circuit. We have demonstrated two different applications using this model. First, we use this model to emulate device behavior in a computational dragonfly model for interception. Second, we have developed a library within the PyTorch framework to add the dendritic circuit component in spiking neural networks (SNNs). Dendrites make SNNs more expressive and improve performance. Current and future work entails further optimizing this library for faster simulation. We are also exploring techniques such as neural ODEs to automate circuit modeling providing useful and fast abstractions.

In our probabilistic exemplar, we use AI-guided codesign techniques like reinforcement learning (RL) and evolutionary optimization (EA) to accelerate device discovery and optimization of probabilistic circuits for true random number generation (tRNG). We leveraged reinforcement learning to optimize device and material properties of a magnetic tunnel junction (MTJ) for a given application task. The RL agent leveraged an abstracted device model of the MTJ to vary key device and material properties for optimal performance. We also utilized evolutionary algorithms to optimize a given tRNG probabilistic circuit for different MTJ device types.

These exemplars demonstrate that codesign tools are important to facilitate cross-pollination and accelerate research across different emerging fields.

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Lattice Boltzmann modelling and study of complex flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LBM MODELLING OF NON-ISOTHERMAL DRYING OF POROUS MEDIA

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ABSTRACT

Convective drying at the pore scale is modelled using a two-component two-phase pseudopotential lattice Boltzmann model (LBM). Two lattice Boltzmann equations are solved, one for liquid water and its vapour and one for dry air. Water vapour is assumed to be well mixed with air forming wet air, while air can also be dissolved in liquid water at low concentration. The approach is shown to be able to model the binary diffusion of vapour and air in the gas phase following Fick's law. The model is validated based on microfluid drying experiments showing good agreement. The LBM model has been extended to non-isothermal conditions, where the heat transport including latent heat is modelled using a finite difference approach and coupled to LBM through the equation of state.

Convective drying of a dual-porosity medium shows two drying regimes, a first drying period at a higher drying rate followed by a second drying period at reduced drying rate. The transition from the first to the second period is observed when capillary pumping from large pores to fine pores at the surface fades out. Based on the capillary pumping principle, we design layered porous media with different pore size and contact angle that guarantee capillary pumping to the surface until low degree of saturation, showing high drying rate and short drying period. The evaporative cooling effect of the wet porous medium during drying is assessed as a potential mechanism in cooling technologies. In real environmental conditions, the convective drying of wet materials, like soils and building materials, may be influenced by solar radiation imposing a temperature gradient. It is found that imposing a temperature gradient can strongly influence the length of the first drying period and the drying rate during the second period.

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Contact and interface mechanics: Modeling and computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NEW PERSPECTIVE ON COMPUTATIONAL CONTACT HOMOGENISATION BASED ON THE METHOD OF MULTISCALE VIRTUAL POWER

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ABSTRACT

Multiscale contact modelling is currently an active research topic which lives in the intersection of the contact mechanics and multiscale analysis spheres. At their core, the so-called contact homogenisation frameworks aim at enriching the macroscopic contact behaviour with information emerging from the highly complex contact interaction at the microscale, underpinned by surface roughness, complex material behaviour, and adhesion, to name a few. While there have been significant efforts to formulate and realise numerical tools that manage multiscale contact, it is still not well-established in the field.

The present work enters the scene with the goal of deriving a contact homogenisation framework bridging microscopic contact and a homogenisation-based constitutive response of the macroscopic interface. Namely, true contact occurs at the roughness level, based on the KKT non-penetration and Coulomb's frictional constraints, and the macroscale does not explicitly enforce contact conditions, yet experiences a contact traction response computed from the microscopic solution. All the theoretical development revolves around the recently proposed Method of Multiscale Virtual Power (MMVP), which provides a systematic approach to developing multiscale theories [1]. The new model is fundamentally characterised by a Minimal Kinematical Restriction based on the carefully selected kinematical postulates. The traction homogenisation formula and the microscopic equilibrium problem are not presumed beforehand, instead coming as consequences of a fundamental multiscale virtual power balance principle. Due to the particular characteristics of the contact problem, novel specialisations of the method to ensure the admissibility of the traction field are proposed and investigated.

The contact homogenisation models are implemented within a large strain finite element program with a dual mortar contact implementation. The formulation is assessed in a series of numerical examples that showcase the overall behaviour of the model, convergence with the dimensions of the microscopic domain and benchmarks with alternatives present in the literature [2,3].

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Multiphase flow and non-Newtonian fluid - Modelling and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INCREASING THE EFFECTIVITY OF OIL AND GAS WELLS' CEMENTING IN CANADA THROUGH MODELLING AND SIMULATION

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ABSTRACT

Primary cementing of oil and gas wells is fundamental to achieve well integrity and prevent leakages, and the thin cement sheath is part of the overall well barrier also used at end of life of the well. Oil leakage, gas migration away from the well, leakage into aquifers are all ecologically damaging occurrences, affecting health and safety, subsurface ecosystems, and local communities. Canada is the world's fifth largest oil producer, has the 3rd largest proven oil reserves and has drilled over 550,000 oil and gas wells. Many wells leak some form of hydrocarbon. Reported leakage rates vary widely according to well type, regulatory jurisdiction, data availability and method of assessment. Dusseault et al. [1] summarize various studies, suggesting ~10% of leaking wells. Since curbing leakage and emissions is beneficial to all and since we are able effectively seal wells, why are we not doing a better job? In other industries, where uncertainty is high and measurement or evaluation difficult, physically-based models and simulations are routinely employed, to fill gaps in understanding, allow exploration of design questions, to use as part of control strategies and guide evaluation. In the oil well industry, two-dimensional (2D) operational simulations provide a level of physical complexity vs computational cost that allows widespread (desktop) computational design usage, yet the tools are not widely available. Our group at UBC has been at the forefront of developing models for primary cementing for over the past 20 years. Our current goal is to bring our models from research codes and laboratory experiments, directly into the hands of Canadian stakeholders, in the form of useable predictive software.

In this talk we will describe our primary cementing models, and our predictive software development project. We model the process as the displacement of viscoplastic fluids in an inclined, non-concentric, narrow annulus. Our 2D model uses a Hele-Shaw approach to describe the displacement, and the Herschel-Bulkley model to describe the fluids. We will overview the evolution of our 2D model, including as a purely laminar, immiscible displacement, the addition of transitional and turbulent regimes, and adding dispersion to the interface to better match our 3D simulations and laboratory experiments results.

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Multi-scale and machine learning-based modeling methods for optimization and design of composites
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTIFIELD MICROMECHANICS ANALYSIS OF COMPOSITES WITH DEFECTS USING CUF

Erasmo Carrera[*1], Alfonso Pagani[1], Marco Petrolo[1], Rebecca Masia[1] and Mattia Trombini[1]*

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ABSTRACT

This work presents the latest developments concerning the micromechanics models built using the Carrera Unified Formulation. CUF is a formulation to obtain any structural theory using a compact notation to define the unknown fields and governing equations. 1D and 2D finite elements based on CUF have proved to be numerically efficient and accurate and may serve as alternatives to 3D elements. For instance, CUF can generate Representative Volume Elements of composite structures and detect the 3D stress field with a fraction of the computational cost required by 3D elements [1]. Micromechanics models from CUF can incorporate defects stemming from manufacturing, e.g., voids, to capture the effect on the local stress and strain fields, including plasticity over the matrix [2].

CUF can be used for multifield analyses [3] as the compact form of the governing equations can be extended to include various fields, e.g., thermal, electrical, magnetical, and combinations thereof. Coupled and uncoupled analyses are possible, and multifield variables can be modeled a priori.
This work focuses on merging the micromechanics and multifield capabilities of CUF for composites. Various numerical examples are considered, e.g., thermo-mechanical analysis of RVE with voids and electromechanical cases. Comparisons with results from the literature are carried out to verify the formulation and assess its numerical efficiency. 3D fields are obtained for different RVE architectures. Perspectives on multiscale analyses are then outlined.

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Modeling and inverse design of architected materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IDENTIFYING WAVE POLARIZATION AND BANDGAPS IN PERIODIC ARCHITECTED MATERIALS

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ABSTRACT

We present a new computational method to accurately identify the elastic wave propagation modes and polarizations in periodic solid structures and metamaterials. The method uses the eigenvectors associated with each propagating wave solution to calculate the contribution of each translational and rotational component of the total mass-in-motion. We use this information to identify the dominant wave propagation mode by defining a relative effective modal mass vector. Then, we associate each wave solution with its correct polarization by defining a polarization factor that quantifies the relative orientation between the wave propagation and lattice motion directions and provides a positive numerical value between 0 (pure S-wave) and 1 (pure P-wave). Further, we suggest a graphical representational scheme for easier visualization of the wave polarization within traditional dispersion plots. To validate the method, we compare our predictions against previously published results for various elastodynamic problems. Finally, we use the proposed method to analyze the effect of various lattice and structural parameter perturbations on the elastic wave propagation and polarized bandgap behavior of a square planar beam lattice. Our analysis reveals the emergence of previously unobserved dynamic characteristics, including various polarized bandgaps, fluid-like behavior, and ultralow-frequency SH- and SV-bandgaps that extend to 0 Hz. Our proposed method provides an alternative computational approach to the typically employed visual mode inspection technique and provides a robust method for analyzing the elastic wave response of periodic solid media.

Advanced numerical techniques for fluid flow in porous media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL SIMULATION OF THE STOKES-BRINKMAN EQUATIONS ON 2D UNSTRUCTURED MESHES USING A MONOLITHIC APPROACH AND A MULTIPOINT FLUX APPROXIMATION METHOD BASED ON HARMONIC POINTS (MPFA-H)

Darlan Carvalho[*1], Pedro Albuquerque[1], Contreras Fernando[1] and Paulo Lyra[1]*

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ABSTRACT

Carbonate petroleum reservoirs are commonly found around the world such as the Brazilian Pre-salt. Due to the nature of the carbonate rocks, diagenetic processes can originate geological features such as vugs, cavities and caves that can be interconnected. These features appear in multiple scales, each influencing the fluid flow inside the reservoir. The presence of these geological features represents a challenge to numerical modeling and simulation of fluid flow in these reservoirs due to the highly heterogeneous rock properties suggesting the use of general unstructured and flexible computacional meshes. Besides, the coexistence of two different flow regimes, a Darcian flow region in the porous media and a free flow region in the vugs, cavities and caves introduces further complexity into the modeling process. In this context, the present work, we propose a cell-centered, collocated, finite volume scheme for the numerical simulation of fluid flow in carbonate petroleum reservoirs. The governing equations are solved using a monolithic approach, where a full pressure support Multipoint Flux Approximation method based on harmonic points (MPFA-H) is extended to discretize Stokes-Brinkman's equations. In our formulation, the pressure gradients are computed via a Global Least-Squares (GLS) approach. Moreover, to guarantee the proper coupling between the pressure and velocity unknowns, a momentum-weighted interpolation method is devised to avoid the odd-even decoupling and non-physical oscillations, typical of collocated approaches. To evaluate the accuracy and robustness o our approach, we have solved some interesting problems found in literature.

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New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION OF UNSTEADY COMPRESSIBLE FLUID FLOWS

Icaro Amorim Carvalho[*1], Diego Hayashi Alonso[1], Luis Fernando Garcia Rodriguez[1] and Emilio Carlos Nelli Silva[1]*

[1]*University of São Paulo*

ABSTRACT

Unsteadiness is closely related with the vortex dynamics that leads to surge and stall. These phenomena and their adverse effects are rooted in vortex shedding – in common with that found in cylinder wakes in laminar and turbulent regimes. Despite previous efforts, the literature still lacks a formulation in topology optimization to evaluate compressible fluid flows that are unsteady, and thus motivates this study. Finite volume simulations are carried out in OpenFOAM to resolve the fluid flow problem efficiently, while a finite element implementation provided by FEniCS computes the sensitivities through automatic differentiation. A combination of the two is found in the FEniCS TopOpt Foam framework which is employed here. Sensitivites obtained through automatic differentiation and finite differences allow to evaluate changes in the vorticity of the domain with respect to the design variable associated with each cell of the domain, that will vary between 0 (solid) and 1 (fluid). The topology optimization method is conducted in this work to address the typical phenomenon of vortex shedding past a circular cylinder in laminar regimes of a Reynolds number of 100: One in incompressible flow; and another in compressible, subsonic regime for a Mach number of 0.5. We specifically envision to attain a final design to minimize the vorticity in the fluid domain and thus attenuate the formation of vortices, present in a multitude of practical applications.

Advances in computational biomechanics and mechanobiology
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NUMERICAL APPROACH TO MODEL THE ROLE OF MECHANICAL STRAIN IN TUMOR GROWTH

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ABSTRACT

Despite significant advances in early diagnosis and treatment solutions, cancer remains the leading cause of death worldwide. Cancer is a malignant pathology characterized by accelerated and uncontrolled cellular proliferation. Several experimental and theoretical efforts have been taken to unravel the mechanism of primary tumor development distant metastasis establishment. Constitutive mechanics models are one of these approaches as they can characterize changes in mass and stress development during tumor growth. From a biomechanical standpoint, solid tumors are hyperelastic, compressible, anisotropic materials with a mechanical behavior both space and time-dependent, whose mass varies over time. Tumor mass increase is a complex phenomenon, influenced by molecular and genetic factors, cell interactions, vascularization, and mechanical cues. The purpose of this work is to provide a numerical framework that incorporates the effect of mechanical strain in tumor growth.
Based on experimental evidence that proliferation is improved in post-stretched cells [1], a constitutive model to describe the strain-driven growth of a mass is developed and implemented into Abaqus® (using a user-defined subroutine) by considering the multiplicative decomposition of the deformation gradient into an elastic and a growth contribution.
The model is initially tested in a simple numerical example (using different deformation modes applied to a single unitary hexahedral finite element) to validate the numerical solution, as well as quadratic convergence and model objectivity. Afterwards, a rectangular specimen, comprised by a solid tumor (with a given preferential growth direction) surrounded by softer tissue, is subjected to cyclic uniaxial and biaxial stretch scenarios. Finally, a case study of the development of a ductal carcinoma in situ (DCIS), a pre-invasive form of breast cancer restricted to the mammary glands' ducts, is performed. Assuming homogeneous nutrient supply, the tumor growth occurs in an anisotropic manner (in the direction of least resistance) influenced by mechanical stimulation (introduced by the contractile myoepithelial cell layer surrounding the duct).
The provided examples demonstrate the potential of the developed model which with a growth evolution law derived by experimental evidence can be a very important tool to better understand tumor growth as mechano-chemo-biological process.

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Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ON THE MODELING OF DAMAGE IN RUBBER-TOUGHENED AMORPHOUS POLYMERS ACCOUNTING FOR CAVITATION AND SHEAR YIELDING

A. Francisca Carvalho Alves[*1], Bernardo P. Ferreira[2] and Francisco Andrade Pires[1]*

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ABSTRACT

Amorphous polymers have been widely used by the scientific and technological communities due to their excellent and versatile performance in several applications, encompassing aeronautics, automotive, structural and electronic industries. Besides their excellent thermal, optical, chemical and mechanical properties, these materials can be easily blended to fulfil specific applications. A well-known and successful example of this blending technique is the inclusion of rubber particles to improve their toughness, such as the acrylonitrile-butadiene-styrene (ABS) binary blend, which combines the amorphous polymer styrene-acrylonitrile (SAN) with rubber-particles.

The rubber particles are responsible for providing the dissipation of energy through different deformation mechanisms, such as cavitation and growth of voids, multiple crazing and shear yielding, and hence promoting the transition from brittle-to-ductile fracture. As a result of the complex synergistic effect associated with these mechanisms, the prediction of their thermomechanical response is not straightforward.

In this context, a novel finite strain visco-elastic visco-plastic constitutive model is proposed to predict the nonlinear response of rubber-toughened amorphous polymers [1], accounting for the nucleation, interaction and growth of voids. A nucleation law is established to predict cavitation under volumetric strains based on a well-established nucleation criterion [2]. A modified version of the well-known Gurson's potential is adopted to capture the void's growth, ensuring the coherence in the energy dissipation between the macro and microscales. A fully implicit integration algorithm is established, and an optimization-based calibration strategy is designed to identify the model's material parameters efficiently. The response of the model is assessed under different triaxial states and is further compared with the homogenized response of a Representative Volume Element of the voided-amorphous polymer microstructure. The results highlight that the model can capture the typical behavior of amorphous polymers, as well as the decrease of stress associated with the increase of the void volume fraction. The efficiency of the calibration procedure and the overall numerical strategy are also demonstrated.

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ANALYSIS OF DENSITY-BASED CELL-SORTING MICROFLUIDIC DEVICES USING A STABILIZED FINITE ELEMENT METHOD

Guillermo Casas[*1], Aniol Sala[1] and Eugenio Oñate[1]*

[1]CIMNE

ABSTRACT

In this work, we use numerical simulations to analyze a class of density-based cell-sorting microfluidic devices. The sorting mechanism exploits (small) density variations among the various particle types using a stratified flow with layers of different densities. This system causes the particles to move toward their equilibrium position under the buoyancy force as they move along the circuit. Previous work on the numerical analysis of such systems has ignored the effect of diffusion, which leads to a blurring of the interfaces between different strata, ultimately affecting the device's precision. We include this effect by numerically solving the convection-diffusion equations to track the evolution of the concentration of the additive used to control the various densities. Other factors, such as the impact of turns in the circuit, are also taken into account. A stabilized finite element formulation is employed to predict the fluid field and the concentration of the additive. We evaluate our numerical results by comparing them to empirical data from the cell separation efficiency of real devices.

Isogeometric methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A COMPARATIVE STUDY OF ASSUMED-STRAIN LOCKING TREATMENTS FOR NURBS-BASED DISCRETIZATIONS

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ABSTRACT

NURBS-based discretizations suffer from the same types of locking as conventional FEA discretizations based on Lagrange polynomials. Locking results not only in smaller displacements and rotations than expected, but also large-amplitude spurious oscillations of the stresses. The large-amplitude spurious oscillations of the stresses can persist for meshes for which the displacements and rotations are already accurate. A direct deployment of the numerical schemes used to overcome locking when using Lagrange polynomials is not an effective strategy to vanquish locking when using NURBS since the levels of continuity across element boundaries of Lagrange polynomials and NURBS are different. Thus, the higher inter-element continuity of NURBS requires the development of new numerical schemes to overcome locking. In this talk, I will compare the performance of different assumed-strain locking treatments for NURBS-based discretizations taking into account both accuracy and computational cost. Specifically, I will consider continuous-assumed-strain (CAS) elements [1, 2], lumped-assumed-strain (LAS) elements [3], Bbar elements, and reconstructed Bbar elements. Second-order and fourth-order structural theories for rods and shells will be studied as well as nearly-incompressible solids. Both linear and nonlinear regimes will be analyzed.

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AN EFFICIENT, HEREDITARY INTEGRAL APPROACH TO MODELING THERMAL AND AGE-INDUCED PERMANENT SET IN POLYMERS

Stephen Castonguay[*1], Joshua Fernandes[21], Michael Puso[1] and Sylvie Aubry[1]*

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ABSTRACT

Polymers often undergo permanent deformation when held under states of strain for extended periods of time, a process that is known as permanent set. The resulting residual strain is a function of both temperature and the amount of time the material spends in a particular strain state. Here, we propose an efficient, hereditary integral method to model this phenomenon. The approach utilizes the transient network framework [1], in which polymer chains can detach from a network and reform in a state of zero stress at the time of re-attachment. Under linear kinetics assumptions, certain simple functional forms for the free energy permit a decomposition of the kernel that allows for a recurrence relationship to be established, bypassing the need to integrate over all time history. Its implementation in a finite element framework is demonstrated for both highly compressible and nearly incompressible material models. Multiple examples are presented which illustrate the effect of varying thermal environments and complex loading histories, as well as the model's ability to handle visco-elasticity at shorter time scales.

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Computational methods for wind energy
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTI-FIDELITY ANALYSIS FOR SITE-SPECIFIC AERODYNAMIC DESIGN OF WIND TURBINE BLADES

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ABSTRACT

The aerodynamic design of wind turbine blades relies on the optimization of blade shapes and profiles, often starting from scaled-up versions of state-of-the-art machines to achieve larger dimensions. The current trend in wind energy development is shifting towards the installation of new plants in deep waters using floating technology. For these novel configurations, the performance requirements for turbines become significantly more stringent, necessitating a considerable increase in specific and rated power while avoiding excessive loads, weights, and hub-heights. Thus, the conventional approach of scaling up machines designed for fixed foundations may no longer be optimal.
In the preliminary design of new blades, aerodynamic calculations are typically entrusted to reduced-order models, often based on the blade element momentum theory (BEMT). These models, developed and refined over the years, are highly performant, offering quick and reliable aerodynamic insights suitable for integration into the aero-servo-elastic analysis of turbines. However, the BEMT-based model has known limitations, especially in determining correct inductions and loads where significant radial flows and viscous effects are present, such as at the blade tip and root regions.
This study proposes a combined approach of high-fidelity and low fidelity modelling to aid in the design of new wind rotor blades for offshore floating applications. The components of the methodology will include 3D computational fluid dynamics analysis based on the Reynolds Averaged Navier Stokes equations solved for the resolved blade shape, a parametric surface definition tool, and adaptive mesh morphing techniques. This system will be interfaced with a design framework that checks performance against characteristic wind conditions at specific target sites using aero-servo-elastic engineering tools.
The goal of this presentation is to describe the new aerodynamic design strategy, its performance, and results, toward the definition of a new optimized blade concepts for specific deepwater sites.

Current trends and advances in enriched finite element methods and coupled simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HIGH-ORDER FORMULATIONS, A POSTERIORI ERROR ESTIMATORS, AND ADAPTIVE PROCEDURES FOR THE G/XFEM

Murilo H. C. Bento[*1], Sergio P. B. Proença[1] and Armando Duarte[2]*

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ABSTRACT

The Generalized/eXtended FEM is able to accurately and efficiently solve problems in which a priori knowledge about their solutions is available. Typical classes of problems in this category are those containing, for instance, weak or strong discontinuities, in the context of either elasticity or heat conduction. The method has proven to deliver well-conditioned and optimally convergent solutions, especially when first-order approximations are considered. Nevertheless, the development of higher-order approximations is ongoing and is of interest due to their higher convergence rates, which give more accurate solutions at a lower cost, and because first-order G/XFEM may be not competitive with second-order FEM for some classes of problems [1], such as those of LEFM. In addition, when it comes to assessing the accuracy of G/XFEM approximations, special tools are needed when exact solutions are not known and a posteriori error estimators play an important role in this. Herein, a newly developed a posteriori error estimator [2], based on a Zienkiewicz-Zhu (ZZ) formulation and tailored to estimate discretization errors of solutions obtained by higher-order G/XFEM [1, 3], is presented. The error estimator is shown to be accurate and computationally efficient through a set of numerical examples. Furthermore, besides being able to estimate well global discretization errors, the estimator is also shown to be locally effective and, therefore, it can be readily applied to drive adaptive simulations. It is known that this type of simulation is important for 3-D LEFM problems since only singular enrichment functions and uniform mesh refinement are not enough to attain optimal convergence [1] and currently, trial and error has been adopted in practical applications to get accurate solutions. Following that, an h-adaptive procedure able to deliver on-the-fly discretizations that meet a pre-specified target on the discretization error and optimal convergence is presented and its advantages are shown.

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Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE FEM AND DPG METHODOLOGY FOR UPSCALING IN SOLID MECHANICS - RECENT ADVANCES

Witold Cecot[1], Marta Oleksy[1] and Marek Klimczak[1]*

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ABSTRACT

The work concerns the development of the Multiscale Finite Element Method (MsFEM) [3] for solid mechanics problems with highly oscillating material coefficients and multifield, high-order FEM approximation stabilized by the DPG methodology.

Our enhancement utilizes static condensation in the domains of coarse elements, previously positively tested for two-dimensional problems [2], which transfers the construction of special (optimal) shape functions (i.e. construction of prolongation operator for heterogeneous materials) exclusively to the interfaces of macro-scale elements. This way, our original interface prolongation reduces both the approximation error and computational costs. Higher-order shape functions enhance the efficiency of calculations, and the DPG methodology [1] ensures discrete stability for the mixed formulation due to on-the-fly constructed optimal test functions. The good accuracy and convergence of the improved method will be illustrated by solutions to selected linear and nonlinear problems in three dimensions. Additional reduction of modeling error may be achieved through several iterations on a fine grid, similar to the multi-grid approach.

In the presentation, we will refer to the statistical approach to upscaling developed by J. T. Oden for modeling contact and friction [4].

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Advanced numerical techniques for fluid flow in porous media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL TREATMENT OF THE COUPLED GEOMECHANICS AND FLUID-FLOW PROBLEM IN CARBONATE ROCKS WITH VUGS

Giovani Cerbato[*1], Hermínio Tasinafo Honório[2], António Fábio Carvalho da Silva[1], Clóvis R. Maliska[1] and Emilio Ernesto Paladino[1]*

[1]*Federal University of Santa Catarina (UFSC)*
[2]*TU Delft*

ABSTRACT

Carbonate are sedimentary rocks that generate significant interest in reservoir engineering, as a substantial amount of the world's hydrocarbon reserves are found in this type of rock. They may be constituted by a porous medium (formed by a liquid/solid phases), as well as vugs (macropores filled with fluid that are relatively larger compared to the pores in the porous medium). In the porous media one has a Darcy's flow and in the vug a Stokes flow. Numerical simulations used to predict fluid flow production in such a rock must consider the coexistence of the flow in the porous medium, the free flow in the vugs, and the mechanical behavior of the rock. In this problem one has two distinct physical regions, and the solution usually employs the Two-Domain Approach[1], which requires boundary conditions at the interface between these two regions, being the major drawback of the approach. An alternative consists of using the same set of equations for both regions, which is referred to as Single-Domain Approach (SDA). In this case, the challenge consists of defining a set of equations that appropriately describes the fluid flow and the geomechanics in both regions. The innovative aspect of this work is the creation of an equation for the geomechanics of the vug region, recalling that the vug is not a rock, and the use of an equation for the fluid flow representing the Darcy equation in the porous media and the Stokes equation on the free fluid flow region. Although SDA eliminates the necessity of boundary conditions between the different domains, it introduces new challenges related to numerical stability. Numerical oscillations in pressure, displacement and fluid velocity field can appear. To overcome this problem, another innovative aspect of this work is the use of Physical Influence Scheme (PIS) for interpolating the solid and the fluid velocities which appears in the mass conservation equation. Results in a rock sample considering a circular vug show that the SDA model with PIS can capture the involved physics producing stable solutions.

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Recent advances in discretization techniques for coupled problems in incompressible fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A HYBRIDIZABLE DISCONTINUOUS GALERKIN APPROXIMATION OF THE DUAL-POROSITY-STOKES PROBLEM

Aycil Cesmelioglu[*1], *Jeonghun Lee*[2], *Sander Rhebergen*[3] *and Dorisa Tabaku*[1]

[1]*Oakland University*
[2]*Baylor University*
[3]*University of Waterloo*

ABSTRACT

In this talk, I will present a numerical method for the dual-porosity-Stokes problem that couples free flow in macrofractures/conduits and flow in microfractures/matrix. Our numerical method couples a pressure-robust IP-HDG method for the Stokes problem and a hybridized BDM discretization for the dual-porosity problem resulting in divergence-conforming velocities and pointwise satisfaction of mass conservation equations in the absence of source terms in the porous medium. A priori error estimates and numerical experiments will be provided.

MACHINE LEARNING-BASED MULTISCALE APPROACH TO ANISOTROPIC DAMAGE IN QUASI-BRITTLE HETEROGENEOUS STRUCTURES

Zakaria Chafia[1], Julien Yvonnet[1] and Jérémy Bleyer[2]*

[1]Gustave Eiffel University
[2]Ecole des Ponts ParisTech

ABSTRACT

A machine learning based multi-scale method is proposed for modeling anisotropic damage in quasi-brittle composite structures. This approach uses the results of damage simulations on Representative Volume Elements (RVEs), at the microscopic scale, as data to build a surrogate model describing the behavior law and internal variables evolution at the macroscopic scale. In order to capture all RVE degradation mechanisms, several damage simulations are performed in a preliminary stage (off-line calculations), at the RVE scale, using the phase field method [1]. Each simulation carried out on the RVE, subjected to periodic boundary conditions, corresponds to a macroscopic strain leading the RVE to its complete state of degradation. At each loading increment, a numerical homogenization technique [2] is applied to evaluate the effective elastic tensor of the RVE. A harmonic analysis of the elastic tensor evolution during crack propagation simulations in the RVE (DDHAD method - Data Driven Harmonic Analysis of Damage [3, 4]) is used to define the macroscopic internal variables. Their evolution is modeled by an appropriate machine-learning-based surrogate model. Machine learning is applied to construct the behavior law and the internal variables evolution, as a surrogate model to be used, at the macroscopic scale. Applications to periodic quasi-brittle composite structures with strongly anisotropic microstructures are presented.

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Scientific deep learning
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DIVIDE AND CONQUER - IMPROVED TRAINING OF NEURAL ORDINARY DIFFERENTIAL EQUATIONS THROUGH TIME-DOMAIN SPLITTING

Dibyajyoti Chakraborty[*1], SeungWhan Chung[2] and Romit Maulik[3]*

[1]*The Pennsylvania State University*
[2]*Lawrence Livermore National Laboratory*
[3]*The Pennsylvania State University, Argonne National Laboratory*

ABSTRACT

Forecasting high-dimensional dynamical systems is a fundamental challenge in various fields, such as geosciences and engineering. Neural Ordinary Differential Equations (NODEs), which combine the power of neural networks and numerical solvers, have emerged as promising tools for forecasting complex nonlinear dynamical systems. However, classical techniques used for NODE optimization are inefficient for learning chaotic dynamical systems. To overcome this limitation, we propose an algorithm splitting the time domain into multiple steps based on the physical properties of the system and penalizing intermediate discontinuities. Our method is devised to address the challenges of non-convexity and exploding gradients observed while optimizing objectives with underlying chaotic dynamics. The proposed algorithm, denoted the Multistep Penalty Neural ODE (MP-NODE), is applied to chaotic systems such as the Kuramoto–Sivashinsky equation and the turbulent forced 2D Navier Stokes equations. It is observed that MP-NODE converges to a better approximation of the physical system for the same training time than standard NODEs. Furthermore, MP-NODE provides performance on par with least-squares shadowing with significant reductions in training costs.

UQ-TTA student paper competition in uncertainty quantification
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DIVIDE AND CONQUER - IMPROVED TRAINING OF NEURAL ORDINARY DIFFERENTIAL EQUATIONS THROUGH TIME-DOMAIN SPLITTING

Dibyajyoti Chakraborty[*1], SeungWhan Chung[2] and Romit Maulik[1]*

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Forecasting high-dimensional dynamical systems is a fundamental challenge in various fields, such as geosciences and engineering. Neural Ordinary Differential Equations (NODEs), which combine the power of neural networks and numerical solvers, have emerged as promising tools for forecasting complex nonlinear dynamical systems. However, classical techniques used for NODE optimization are inefficient for learning chaotic dynamical systems. To overcome this limitation, we propose an algorithm splitting the time domain into multiple steps based on the physical properties of the system and penalizing intermediate discontinuities. Our method is devised to address the challenges of non-convexity and exploding gradients observed while optimizing objectives with underlying chaotic dynamics. The proposed algorithm, denoted the Multistep Penalty Neural ODE (MP-NODE), is applied to chaotic systems such as the Kuramoto–Sivashinsky equation and the turbulent forced 2D Navier Stokes equations. It is observed that MP-NODE converges to a better approximation of the physical system for the same training time than standard NODEs. Furthermore, MP-NODE provides performance on par with least-squares shadowing with significant reductions in training costs.

SciML in the real world
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BAYESIAN DISCOVERY OF INTERPRETABLE STOCHASTIC PARTIAL DIFFERENTIAL EQUATIONS FROM LIMITED AND NOISY DATA

Tapas Tripura[1] and Souvik Chakraborty[*1]*

[1]Indian Institute of Technology Delhi

ABSTRACT

Data-driven discovery of governing physics of dynamical systems in terms of ordinary and partial differential equations (ODEs/PDEs) has become an exciting area of scientific machine learning [1]. In complex dynamical systems where the complete knowledge of underlying governing laws is not known a priori, the data-driven frameworks provide an effective way of distilling the governing equations of motion. However, all natural dynamical systems are stochastic in nature due to the continuous interaction between the dynamical system and the external stochastic environment. The approaches to discovering ODEs/PDEs completely neglect the stochasticity in the physical dynamical systems. Of late, a few studies have been carried out to discover interpretable stochastic differential equations (SDEs) from data [2]. An effective method for discovering interpretable equations of motion of stochastic continuous systems from data is still missing in the literature. To that end, we propose a novel data-driven framework for discovering Stochastic Partial Differential Equations (SPDEs) in this study. We propose the extended Kramers–Moyal expansion to express the deterministic and stochastic parts of SPDEs using state observations. We introduce a sparse Bayesian learning (SBL) framework for discovering a sparse representation of the deterministic and stochastic components of SPDEs from data. For efficient SBL, we employ the variational Bayes inference with Spike-and-Slab prior. This setup not only promotes sparsity in the discovered SPDE but also helps in avoiding overfitting of the discovered interpretable model. We illustrate the fidelity of the proposed SPDEs discovery framework for rediscovering the governing equation of the (a) stochastic heat equation, (b) stochastic Allen–Cahn equation, and (c) stochastic Nagumo equation from 1-2 seconds of state measurements. The rediscovered SPDEs show an accurate identification of the true governing equations. In the low data limit, the ability of the proposed Bayesian framework to quantify uncertainty in the discovered model is an additional advantage. We illustrated the application of the developed framework in time-dependent reliability analysis of aging structures. Other potential applications of the developed framework include atomistic modeling, mechanical systems, climate modeling, and financial forecasting.

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Uncertainty quantification and reliability analysis in engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INTREPID MCMC: A NOVEL SAMPLING ALGORITHM FOR BETTER EXPLORATION AND IDENTIFICATION OF DISJOINT FAILURE REGIONS IN SUBSET SIMULATION

Promit Chakroborty[*1] and Michael Shields*[1]

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ABSTRACT

Estimating the reliability of real-world infrastructure requires multiple evaluations of computational models that are often highly complex and time-consuming. For such problems, Subset Simulation (SuS, introduced by Au and Beck in 2001) has been an invaluable tool. Traditionally, SuS uses simple random-walk MCMC algorithms such as the Metropolis-Hastings or Component-wise Metropolis-Hastings methods to generate samples from the conditional distributions relevant to the problem. However, various blind spots of the SuS framework have been recognized under this paradigm, leading to non-convergence or false convergence of the target failure probabilities. In this work, we propose a novel random-walk MCMC sampling scheme, called Intrepid MCMC, that is specifically designed to improve the ability of the Markov Chains to explore the parameter space, by randomly sampling in regions of the distribution tails that cannot normally be reached by traditional MCMC methods due to the additional response-function dictated rejection step utilized by Subset Simulation. The underlying intuition is discussed, followed by a case study highlighting the ability of Intrepid MCMC to find failure regions that are missed by traditional Subset Simulation implementations.

UQ-TTA student paper competition in uncertainty quantification
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INTREPID MCMC: A NOVEL SAMPLING ALGORITHM FOR BETTER EXPLORATION AND IDENTIFICATION OF DISJOINT FAILURE REGIONS IN SUBSET SIMULATION

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Estimating the reliability of real-world infrastructure requires multiple evaluations of computational models that are often highly complex and time-consuming. For such problems, Subset Simulation (SuS, introduced by Au and Beck in 2001) has been an invaluable tool. Traditionally, SuS uses simple random-walk MCMC algorithms such as the Metropolis-Hastings or Component-wise Metropolis-Hastings methods to generate samples from the conditional distributions relevant to the problem. However, various blind spots of the SuS framework have been recognized under this paradigm, leading to non-convergence or false convergence of the target failure probabilities. In this work, we propose a novel random-walk MCMC sampling scheme, called Intrepid MCMC, that is specifically designed to improve the ability of the Markov Chains to explore the parameter space, by randomly sampling in regions of the distribution tails that cannot normally be reached by traditional MCMC methods due to the additional response-function dictated rejection step utilized by Subset Simulation. The underlying intuition is discussed, followed by a case study highlighting the ability of Intrepid MCMC to find failure regions that are missed by traditional Subset Simulation implementations.

Certification of simulations and model adaptation in computational science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADAPTIVE MODELING AND LEARNING OF MATERIAL LAWS FOR EFFECTIVE DATA ASSIMILATION

Ludovic Chamoin[*1], Antoine Benady[1], Sahar Farahbakhsh[1], Emmanuel Baranger[1] and Martin Poncelet[1]*

[1]ENS Paris-Saclay

ABSTRACT

In the context of data assimilation, selecting a model which is consistent with the richness of data is a fundamental issue. On the one hand, the model should not be too crude, so that it is able to reproduce the physics revealed by data. On the other hand, it should not be too complex as this would lead to useless computational effort faced to limited experimental information and measurement noise. We propose here a methodology that permits automatic model selection and adaptivity when comparing model outputs and observations. It employs the concept of modified Constitutive Relation Error (mCRE) that refers to reliability of information. This concept has been used for model updating in many structural mechanics applications, and it is here advantageously employed to qualify and adapt the model complexity (by means of a natural modeling error indicator provided by mCRE). We will show how this permits to perform adaptive modeling with local higher complexity when localized physical phenomena (such as damage) occur, in order to manage computation and experimental resources at best. This goes with the selection of a suitable model in a hierarchical list, and with the adaptation of the model parameter space (e.g. refinement of the mesh used to describe a parameter field).

We will also show how the mcRE concept can be coupled with data-based enrichment of the model structure using deep learning tools. The idea here is to learn and correct model bias; it refers to hybrid twins and physics-constrained neural networks which have received much attention in recent years. A method using neural networks for learning constitutive laws in the form of thermodynamic potentials is proposed, with an associated loss function built from the mCRE functional.
All developments will be illustrated on various numerical experiments involving synthetic or real experimental data.

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H-N. Nguyen, L. Chamoin, Model and mesh selection from a mCRE functional in the context of model identification with full-field measurements, submitted, 2023

M. Diaz, P-E. Charbonnel, L. Chamoin, Fully automated model updating framework for damage detection based on the modified Constitutive Relation Error, Computational Mechanics, online, 2023

This project has received funding from the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation programme (grant agreement No. 101002857)

Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SOME RECENT ADVANCES IN STRUCTURAL DAMAGE TRACKING AND MONITORING

Ludovic Chamoin[*1], Sahar Farahbakhsh*[*1], Matthieu Diaz[2], Martin Poncelet[1] and Pierre-Etienne Charbonnel[3]*

[1]ENS Paris-Saclay
[2]EDF
[3]CEA

ABSTRACT

Damage tracking and monitoring from digital twins and in situ measurements, through the DDDAS framework, has been one of the numerous research topics addressed by J.T. Oden. In his memory, the talk will present some recent developments on this critical issue, which aim to design smart and autonomous mechanical structures able to perform online control of their health and take anticipated actions during service. An innovative cross-disciplinary approach will thus be presented, which performs fast sequential data assimilation from hybrid twins. This approach couples several advanced numerical methods such as model reduction, adaptive modeling, or Kalman filtering, together with a specific cost function which brings robustness faced to highly nonlinear models, various uncertainty sources, and real-time computation constraints. Its capabilities will be shown on several practical engineering applications when inferring real data on-the-fly and performing online health monitoring on large scale structures.

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L. Chamoin, E. Baranger, A. Bénady, P-E. Charbonnel, M. Diaz, S. Farahbakhsh, L. Fribourg, D. Martin-Xavier, M. Poncelet, A novel DDDAS architecture combining advanced sensing and simulation technologies for effective real-time structural health monitoring, Handbook of Dynamic Data Driven Application Systems, Springer (to appear)

M. Diaz, P-E. Charbonnel, L. Chamoin, Fully automated model updating framework for damage detection based on the modified Constitutive Relation Error, Computational Mechanics, online, 2023

This project has received funding from the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation programme (grant agreement No. 101002857)

Theory and application of provably-robust and efficient high-order methods for high-fidelity computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ENFORCING CELL ENTROPY INEQUALITIES USING SUBCELL LIMITING

Jesse Chan[*1] and Yimin Lin*[12]

[1]*Rice University*
[2]*Applied Intuition*

ABSTRACT

Subcell limiting strategies for discontinuous Galerkin spectral element methods do not naturally satisfy a semi-discrete cell entropy inequality. In this work, we introduce a subcell limiting strategy that satisfies a semi-discrete cell entropy inequality by formulating the limiting factors as solutions to an optimization problem whose exact solution can be computed via a greedy algorithm. We also discuss how the proposed subcell limiting strategy can be modified to accommodate general convex constraints. Numerical experiments suggest that the proposed limiting strategy preserves high-order accuracy for smooth solutions and converge to entropic solutions.

SPATIAL AND TEMPORAL COUPLING METHODS FOR THE MODELLING OF WAVE PROPAGATION IN HETEROGENEOUS MEDIA

Kin Fung Chan[1], Nicola Bombace[2], Indrajeet Sahu[1], Simone Falco[1] and Nik Petrinic[1]*

[1]*University of Oxford*
[2]*AMD*

ABSTRACT

The discretisation of structures in space and time is directly related to the accuracy of the finite element method when modelling wave propagation. However, utilising a very fine mesh, and a single time step across an entire domain may be computationally inefficient. Firstly, this work proposes a technique for the explicit coupling of non-matching meshes, without the use of Lagrange multipliers and solving an additional system of equations. We employ an analytical method of finding the shape functions on any quadrilateral surface, followed by the transfer of nodal masses and internal forces on a coupling interface. Through enforcing the continuity of acceleration between subdomains, stability is ensured. The method obeys the conservation of mass and internal energy between subdomains. Should a subdomain be discretised with too coarse a mesh, we highlight the issue of spurious wave reflection when conventionally modelling high frequency waves. We also present a novel multi time stepping algorithm, in an updated Lagrangian formulation, that allows for subdomains to independently advance through time. Unlike existing algorithms, we do not assume a constant or integer ratio between coarse and fine temporal discretisations. Both algorithms allow for the concurrent coupling of several subdomains, each with their own mesh and respective time step. The algorithms are demonstrated in three dimensions, where subdomains can be meshed independently with their own element formulation. Wave propagation in Metaconcrete is studied numerically, demonstrating a large speed up when simulating metamaterials in comparison to monolithic simulations. We also study polycrystalline materials, where individual grains have their own spatial and temporal discretisation.

Fracture, damage and failure mechanics of cementitious materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREDICTING THE MECHANICAL PROPERTIES OF CONCRETE MATERIALS BY MULTISCALE MODELING

Mei Chandler[*1], Mark Adley[1], William Lawrimore[1], Andrew Bowman[2], Micael Edwards[1], Robert Moser[1] and Zackery McClelland[1]*

[1]*The U.S. Army Engineer Research and Development Center*
[2]*U.S. Army Engineer Research and Development Center*

ABSTRACT

Concrete materials are inherently heterogeneous and include internal structures and constituents across length scales ranging from nanometers to tens of millimeters. Multiscale structures and constituents of concrete materials include heterogeneities such as aggregates, sand, fibers, voids, and cracks. The properties and responses of concrete under different loading conditions are dependent upon the multiscale structures and the properties of constituents.

In this work, a hierarchical multiscale finite element modeling method was developed to predict the properties of concrete materials based on their mix designs and experimental paste properties. Properties of fine and coarse aggregates were not experimentally tested, and were estimated based on limited geological information. Nonetheless, the predicted concrete properties closely matched the experimental results for various loading conditions, such as unconfined uniaxial compression, triaxial compression under different confining pressures, and hydrostatic and uniaxial strain compression. The method presented provides a virtual platform for predicting concrete material properties and designing concrete materials for structural applications.

Permission to publish was granted by the Director, US Army Engineer Research and Development Center, Geotechnical and Structures Laboratory.

Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT OF MIXED MATERIAL POINT METHOD FOR ANALYSIS OF FREE-SURFACE AND SEEPAGE FLOW

Bodhinanda Chandra[*1], Ryota Hashimoto[2], Ken Kamrin[3] and Kenichi Soga[1]*

[1]*University of California, Berkeley*
[2]*Kyoto University*
[3]*Massachusetts Institute of Technology*

ABSTRACT

The Material Point Method (MPM) has been widely developed in the past decades for simulating large deformation in solids and geomaterials. However, the method still faces significant challenges in simulating incompressible flow due to three major issues: (i) volumetric locking due to the incompressibility constraint, (ii) the accumulation of quadrature errors, and (iii) instabilities induced by the transfer of information between particles and background grids. Aiming to address these issues, the current research develops a novel stabilized mixed MPM [1] for both free-surface and seepage flow [2]. Unlike traditional Eulerian CFD solvers, the proposed mixed MPM employs a monolithic displacement-pressure formulation inspired by the mixed-form updated-Lagrangian Finite Element Method (FEM). By coupling the displacement and pressure fields and solving them concurrently, the developed solver eliminates the need for free-surface pressure detection and imposition, distinguishing it from the typical fractional-step method. This attribute effectively mitigates spurious pressure oscillations that often arise in MPM from switching free-surface nodal pressure imposition on and off as the fluid front moves through the background grid. Furthermore, to ensure numerical stability, the variational multiscale method (VMS) is incorporated to satisfy the discrete inf-sup stability condition. To simplify the balance equations, a unified formulation to integrate the Navier-Stokes equation with the Darcy-Brinkman-Forchheimer equation is proposed. This unified formulation is then integrated with a blurred interface approach, resulting in a seamless transition of flows between free and porous domains, as well as across two distinct porous media. The proposed formulation's efficacy is verified through benchmark cases in 1D, 2D, and 3D scenarios. A comprehensive verification suite, including analytical solutions for 1D gravity-driven flows under various conditions, is derived to verify the accuracy of the method. Further numerical benchmarks and experiments also demonstrate enhanced accuracy and stability compared to analytical, experimental, and other numerical methods.

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Advances in material model calibration for computational solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE MODELING OF ACTIVE BRAZING

Michael Chandross[*1], Ian Winter[1], Eric Rothchild[1], Jaideep Ray[1], Edward Arata[1], Ping Lu[1], Jeffrey Horner[1], Scott Roberts[1], David Kemmenoe[1], Anthony McMaster[1] and Anne Grillet[1]*

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ABSTRACT

Active brazing is a high temperature joining method that is often used to make hermetic joints between dissimilar materials, like metals and ceramics. A common issue in active brazing is run-out that occurs when a wetting instability causes the braze alloy to flow out of the joint. The spreading is controlled by the wetting of the two substrates by the braze alloy, and this is directly related to the thermodynamic properties of the materials and interfaces, namely (a) surface energies of the solids, (b) surface tension of the liquid braze alloy and (c) the interfacial energies between them. If these quantities are known, then the wetting angles can be predicted using Young's equation. Understanding how these energies vary as a function of composition and temperature is crucial for designing a high quality braze process, but these quantities are hard to measure experimentally. Atomistic simulations provide a route for determining these energies, but methods for treating the metals and the ceramics in the same model are difficult to parameterize and computationally expensive. We present results of a newly developed reactive force field able to accurately model brazing of a model steel to alumina with a AgZr alloy. The brazing is essentially a three step process in which (1) Zr migrates to the alumina surface, and scavenges oxygen to form a ZrO2 surface layer (2) liberated Al diffuses through the braze alloy to the steel surface where extensive mixing of the liquid and solid metals form a multicomponent alloy and (3) the (predominantly) Ag braze alloy wets the two surfaces to form the final joint. We present the results of atomistic simulations aimed at accurately representing the full braze process, including reactions and wetting at both the ceramic and metal surfaces. Surface and interfacial energies are computed using thermodynamic integration to avoid the excessive run times (> 150 ns) necessary for direct wetting simulations. We demonstrate that after calculating these energies Young's equation accurately predicts the wetting angle for a variety of materials. Finally, we use the atomistic simulations to develop a data-driven constitutive model that is implemented in a finite element code to simulate the full brazing process at the manufacturing scale. Results from the simulations are compared to experiments, and the conditions that lead to run-out will be discussed.

Recent advances in indirect structural health monitoring
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PRELIMINARY STUDY OF VEHICLE-BRIDGE INTERACTION USING INSTANTANEOUS FREQUENCY RESPONSE FUNCTIONS

Chia-Ming Chang[*1] and Chi Cheng*[1]

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ABSTRACT

When a vehicle travels on a bridge, the interaction generated between the vehicle and the bridge is the main source of dynamic response in the system. If the frequencies and energy of the bridge, vehicle, and external forces fall within a specific range, excessive deformation of the bridge can be found, leading to damage or other safety issues. In previous studies, the vehicle scanning method was mainly used to indirectly estimate the natural frequencies of the bridge and yielded corresponding structural monitoring methods. However, this method cannot determine the impact of the parameters of the vehicle-bridge interaction from both energy and frequency relationships. Therefore, to understand the characteristics and behavior of the vehicle-bridge interaction system, this study derives the instantaneous frequency response function of the system. In this research, a single sprung mass or multiple sprung masses are used to simulate the moving train. The assumed mode method is applied to simulate the bridge response in the form of the first mode or the superposition of multiple modes. Subsequently, the equation of motion of the vehicle-bridge interaction is established and converted into the frequency domain by the Fourier transform. Eventually, the instantaneous frequency response function of the vehicle-bridge interaction is obtained. In this research, a parametric study is carried out to investigate multiple variables (i.e., mass ratios between the vehicle and bridge, vehicle stiffness, bridge lengths, vehicle speeds, and number of modes and sprung masses), and these results are compared to the finite element analysis and a previous study in literature. As a result, the analytically instantaneous frequency response function is validated to be consistent with numerical results, and this instantaneous frequency response function has the potential to be employed in the structural monitoring of bridges in the future.

Microstructures of chemically complex materials and their impacts on material properties from multiscale simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RANDOM SOLUTE DISTRIBUTION EFFECT ON MECHANICAL BEHAVIOR IN HIGH-ENTROPY ALLOYS: A CRYSTAL PLASTICITY FINITE ELEMENT STUDY

Hsuan-Wu Chang[*1], Wei-Chih Huang[1], Chang-Wei Huang[2] and Yu-Chieh Lo[1]*

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ABSTRACT

High-entropy alloys, a new type of alloy composed of multiple primary elements, present interesting mechanical properties due to the random distribution of solutes. This randomness leads to varying energy barriers for dislocation movement, making the process less predictable and causing fluctuations in the overall plastic deformation behavior. This study combines the theory of dislocation density crystal plasticity with the characteristic randomness of solutes. Through a high-entropy alloy finite element model, we introduce a random factor into the parameters of statistically stored dislocations. Utilizing the fine-division capabilities of the finite element method, we establish multiple sets of models for tension testing. By analyzing the resulting stress-strain curves, we aim to simulate and investigate the mechanical properties of high-entropy alloys with solute randomness. This approach allows us to observe mesoscale behavior and explore the influence of solute randomness range on the overall model.

Improving the efficiency and accuracy of computational methods through machine learning
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A TWO-DIMENSIONAL SHOCK WAVE PATTERN RECOGNITION ALGORITHM BASED ON CLUSTER ANALYSIS

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ABSTRACT

A new technique for detecting and recognizing two-dimensional shock wave interaction patterns in compressible, inviscid flow solutions computed by shock-capturing solvers is proposed. The implementation process of this algorithm is illustrated from three aspects in detail. First, using a traditional shock wave detection approach based on local flow parameters, a series of grid-cells near the shock waves are identified. Next, the shock cells are divided into various clusters by means of a classical K-means clustering algorithm, and the category of each cluster will be defined according to its adjacent information. Finally, a criterion is introduced to merge related adjacent clusters and further determine the locations of shock interaction points; the clusters contained in each shock wave are recorded, and then all the fitting shock lines can be obtained by the Bézier curve fit algorithm. Numerical experiments show that this newly developed technique can be used under different types of meshes, and the fitted shock lines have high quality and positional accuracy; meanwhile, the multiple shock wave interaction patterns are clearly recognized, which can also provide a good visualization method for analyzing the motion and evolution of shock waves in complex, unsteady flow.

Scientific machine learning for geophysical applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CLASSIFICATION OF INFRASONIC SIGNALS OF TATUN VOLCANO GROUP WITH UNSUPERVISED MACHINE LEARNING

Wei-Tze Chang[*1], Yin-Cherng Lin[2], Ya-Chuan Lai[1], Min-Hung Shih[1], Jye-Hwang Lo[1], Cheng-Horng Lin Lin[3], Jen-Yu Han[4] and Chuin-Shan Chen[4]*

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ABSTRACT

Infrasonic signals of large fumarole fields imply important information related to volcanic activities, which directly reflects the changes in the state of the magma or hydrothermal system underground. Variations in the number, type, location, and magnitude of fumarole activities may indicate volcanic anomalies. However, infrasonic signals can be caused by other events, such as earthquakes, gusts, extreme weather, and even human activities, which are difficult to process and identify. This research studied the records of 11 infrasonic sites around the Tatun Volcano Group (TVG) in Taiwan. The signals were transformed into the frequency domain via the Fast Fourier Transform (FFT) to understand its characters. To overcome the uncertainty of infrasonic signals in both time and frequency ranges, the records were then transformed into the Power Spectral Density (PSD) as the basis for analysis. This is due to the PSD representing the power content in a specific time and frequency range. This makes it easier to be superposed with any other PSD in small segments of time and frequency ranges. Two clustering methods, the k-means clustering and the Density-Based Spatial Clustering of Applications with Noise (DBSCAN), were used to achieve unsupervised machine learning of the critical feature of PSD to identify the special events of the volcano. The research results will be transformed into an automatic TVG platform for real-time monitoring, simplifying the significant data for geoscience experts.

INTEGRATING MECHANICS INTO MACHINE LEARNING FOR ELASTOPLASTIC BEHAVIOR MODELING IN FIBER-REINFORCED COMPOSITES

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ABSTRACT

The fiber-reinforced composites are widely used in aerospace, automotive industries and medical area due to its distinguished properties, and its complex three-dimensional elastoplastic behavior can be modeled by machine learning (ML). However, the significantly reliance on substantial training databases hinders progress in ML modeling.To overcome this challenge, our research introduces an innovative mechanics-informed ML approach, aiming to advance the predictive accuracy of the elastoplastic behaviors of unidirectional FRC with a limited database. Incorporating a stress and strain decomposition method rooted in mechanical invariant theory, we establish two parallel Artificial Neural Networks (ANNs) to articulate deviatoric behaviors and the coupling of volumetric and fiber-directional behaviors respectively.The mechanics-informed approach streamlines the architecture of the ANNs, requiring only two inputs and two outputs for each ANN, in contrast to the conventional six-dimensional strain and stress tensors. This reduction in input dimensions significantly enhances predictive accuracy, even with a limited database. Additionally, a tensor transformation link for the output stress of ANNs is incorporated, ultimately deriving tensor-valued stress. Furthermore, our ML approach is refined to predict the impact of the loading path, ensuring a more comprehensive elastoplastic behavior modeling. To validate our proposed ML-based constitutive model, we conduct direct numerical simulations (DNSs) based on a representative volume element, generating datasets for model training and validation. Comparative analysis of results obtained through DNS and ML showcases the exceptional predictive accuracy of our proposed model, even with a small training database.

Data-driven modeling and design of materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN-MULTISCALE MODELING OF ANISOTROPIC DAMAGE FROM RVE FRACTURE SIMULATIONS

Julien Yvonnet[1], Qi-Chang He[1], Pengfei Li[1] and Souhail Chaouch[1]*

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ABSTRACT

A data-driven approach is proposed to construct anisotropic damage models with a minimal number of internal variables from phase field - crack propagation simulations on Representative Volume Elements (RVEs) of quasi-brittle materials. The approach resorts in particular to a harmonic analysis of damage. The orientation distribution functions of two elastic moduli are numerically determined while accounting for the effects of the nucleation and propagation of microcracks by the phase field method. Given these two functions, the effective elastic tensor of a material without or with microcracks is uniquely determined. The expansions into two Fourier series of the relative variations of these two functions related to an undamaged reference state and to a damage state make appear damage internal variables naturally. The number and natures of these variables can be optimized by truncating the Fourier series according to the degree of approximation desired and using POD (Proper Orthogonal Decomposition). Thus, 2D and 3D anisotropic damage models can be constructed without resorting to usual assumptions made in damage mechanics. This construction holds for complex microstructures including image-based ones and for arbitrary loading history. 2D and 3D applications are provided to evaluate the accuracy of the damage models constructed and to show the potential of the approach proposed.

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MACRO CLUSTERING FOR ACCELERATING FE2 MULTISCALE SIMULATIONS OF NONLINEAR COMPOSITES CONSIDERING ELASTOPLASTICITY, VISCOELASTICITY AND DAMAGE

Souhail Chaouch[*1] and Julien Yvonnet*[1]

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ABSTRACT

FE2 method [1] is one of the most accurate widespread approaches for multi-scale modeling of nonlinear heterogeneous materials. In this technique, a macroscopic problem is discretized into a number of finite elements, the constitutive law of each element is assumed to be unknown, and is obtained numerically by solving a nonlinear representative elementary volume (RVE) problem at each macroscopic Gauss point. On the microscopic scale, an RVE is defined and discretized into finite elements too. The main inconvenient of this approach is the involvement of high computational cost, which limits its feasibility for industrial applications.

A method based on unsupervised machine learning is developed to overcome this problem [2]. The idea is to cluster macroscopic integration points in the macro mesh having close mechanical states. Then, instead of solving one nonlinear RVE problem for each Gauss point, only one nonlinear problem is solved for each group of integration points. This procedure significantly reduces the number of RVEs problems to be solved in each Newton iteration at the macro scale.

Several important improvements are made to this method labeled KMFE2 in [3]. First, the definition of macroscopic stress within each cluster is extended using linear interpolation in stress-strain space. Then, the number of clusters is considerably reduced in the case of the presence of internal variables as compared to the previous technique developed in [2]. Finally, some convergence issues associated with the use of clusters are addressed.

This technique has been successfully applied to two-dimensional applications using different loading behaviors and boundary conditions. It is applied to different composite materials with 1) hyperelastic properties, 2) viscoelastic properties, and 3) elastoplastic properties. Finally, extensions of the method to damage are discussed. Typical speed-up factors of around 20 compared to the classic FE2 method were observed, even though no learning step, data base construction or off-line calculations are required.

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Computational models and methods for predicting cancer progression and treatment response
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BUILDING TRUST IN CANCER-PATIENT DIGITAL TWINS FOR PERSONALIZED TREATMENT PLANS

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ABSTRACT

This talk focuses on the mathematical and computational ingredients needed to grow trust in patient-specific digital twins. We build on the work in Refs. [1,2] that developed the mathematical foundations of a predictive digital twin as a probabilistic graphical model, encoding uncertainty as a core part of the digital twin model and using Bayesian methods to execute the digital twin's calibration, prediction, and decision tasks. In this work, we consider a digital twin supporting a human decision-maker for risk-aware clinical decision-making in brain cancer. To achieve appropriate level of trust, the patient-specific digital twin should be able to (i) provide interpretable decisions with explainability of underlying models being key, (ii) quantify the effects of multiple sources of uncertainty and account for underlying risk in safety critical decisions, and (iii) be computable on actionable (possibly real-time) time scales. We achieve explainability and interpretability through a model-centric view of the digital twin that places physics-based models at the core. This leads the digital twin parameters to have interpretable physical meanings, and the sensitivities that drive the digital twin predictions/decisions to be related to some physical phenomena. The predictive digital twins are made patient-specific through continuous calibration using the patient's data and are deployed for forecasting with quantified uncertainty under different control actions. As shown in Ref. [2], we then solve the optimal control under uncertainty problem balancing treatment efficacy and toxicity that leads to a suite of risk-informed decisions for the particular patient. In order for these decisions to be useful for the clinicians, the digital twin needs to be executed within acceptable time-scales. We achieve fast computations through the use of explainable surrogate models and integration of multiple information sources of varying fidelity and cost in a multifidelity setting.

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Imaging and computational methods for biomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFICIENCY AND ACCURACY IN LARGE-SCALE CARDIAC SIMULATIONS WITH COMPRESSED COMMUNICATION AND ALGEBRAIC ADAPTIVITY IN BDDC PRECONDITIONERS

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ABSTRACT

Cardiac electrophysiology simulations are essential for understanding arrhythmia mechanisms and designing effective treatments. Large-scale problems in this domain, characterized by elliptic and parabolic equations, necessitate efficient parallel preconditioners, particularly in the context of domain decomposition. Additionally, the locality of solution features in cardiac electrophysiology simulations calls for adaptive methods. However, traditional mesh refinement and coarsening approaches incur significant overhead. This study contributes novel solutions to address these challenges in distributed computation for cardiac simulations with cellular resolution.

The cardiac extracellular-membrane-intracellular (EMI) model enables the precise geometrical representation and resolution of aggregates of individual myocytes. Achieving efficient higher-order time stepping becomes imperative due to large problem sizes. We consider algebraic adaptivity, i.e. nested subset selection for degrees of freedom in spectral deferred correction methods (SDC)~\cite{CheginiSteinkeWesier}. Shrinking the effective support of SDC corrections allows for a reduction of the spatial domains on which Euler subproblems need to be solved, instead of computing on the whole domain. Improved speedups are obtained by the ladder method, using coarser collocation grids on the first sweeps in the SDC computations, method~\cite{CheginiSteinkeWesier}. However, the Balancing Domain Decomposition by Constraints (BDDC) preconditioner~\cite{Mai} requires expensive reconstruction if the basic time step or degree of freedom set changes. We propose a novel combination of BDDC and algebraic adaptivity, demonstrating computational efficiency in numerical examples. The approach involves a subdomain-wise subset selection, enabling an efficient combination with BDDC and incurring negligible overhead.

Distributed solvers such as the BDDC preconditioner, need to exchange data between compute nodes, which can become a bottleneck in massively parallel computations. We explore lossy compression~\cite{wesierCompress}, such as transform coding, quantization, and optional entropy coding, to reduce data exchanged between adjacent subdomains. While providing effective solutions, this approach introduces computational overhead, latency, and errors, dependent on quantization. We present accuracy models and identify scenarios where lossy compression proves beneficial, supported by practical numerical experiments.

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Microstructures of chemically complex materials and their impacts on material properties from multiscale simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PLANAR FAULT TRANSFORMATION AND UNFAULTING OF INTERSTITIAL DISLOCATION LOOPS IN IRRADIATED CHEMICALLY COMPLEX INTERMETALLIC ALLOYS

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ABSTRACT

The present study has systematically investigated unfaulting mechanism of single-layer interstitial dislocation Loops (IDLs) in irradiated FCC-(Ni,Al), L12-(Ni3Al,Ni3Fe) to extend the existing unfaulting theory from pristine FCC lattice to the L12 ordered lattice, employing atomistic simulations combining continuum theory. Two types of variants for the IDLs have been determined with different superlattice planar faults enclosed in the Frank loop. The unfaulting routes of IDLs by Shockley partial loops have been unveiled through examining the energy barriers of superlattice planar fault transformation. The symmetry breaking occurring in the unfaulting processes were further elucidated and summarized. A continuum model has been formulated to enable quantitative theoretical analysis of the energetics of IDLs and prediction of the unfaulting threshold. These findings clarify the effects of complex faults and symmetry breaking on unfaulting behaviors of IDLs in irradiated L12-(Ni3Al, Ni3Fe), and could be transferable to other L12 systems, and more generally, other chemically complex intermetallic alloys.

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Advanced machine learning methods for multiscale modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BIOMECHANICS ANALYSIS BASED ON HIGH-RESOLUTION LIVE MICRO-CT IMAGES IN THE RAT TEMPOROMANDIBULAR JOINT

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ABSTRACT

The mandible bones feature complex trabecular bone structures and various muscles, resulting in complicated hinge and sliding motions, playing an important role in both humans and rats. Existing numerical models in the literature typically simplify loading conditions and adopt uniform bone properties. In this study, a finite element model of a rat's mandible using micro-CT images at three resolutions (20, 40, and 80 μm) is constructed. Where material properties for each element in the model were mapped based on the brightness of the corresponding pixel in the micro-CT image, revealing a detailed trabecular bone structure. Bio-realistic loads, accounting for the surrounding muscles and biting force on the teeth, which aligns with the anatomical and experimental data, were applied as the boundary conditions, simulating the rat chewing process. The resulting stress distribution in the mandible and temporomandibular joint is in good agreement with experimental observations. Furthermore, it is worth noting that the models generated at different resolutions yielded varying numerical results. This also suggests the most suitable image resolution for the rat’s mandible, considering that higher resolution also entails higher radiation exposure. This work establishes a comprehensive workflow for generating a bio-realistic numerical model with enhanced validity, contributing to the refinement of mandible biomechanics studies.

New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION FOR PARTICLE FLOW USING EULERIAN-EULERIAN MODEL WITH A FINITE DIFFERENCE SCHEME

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ABSTRACT

Topology optimization is a powerful tool to generate an optimal configuration for various engineering problems. For particle flow problems, some studies on topology optimization for single-particle behavior using an Eulerian-Lagrange model have been presented [1]. In this study, we propose a topology optimization method for dispersed particle flow based on an Eulerian-Eulerian model using an implicit finite difference flow solver [2]. In the optimization procedure, we employ automatic differentiation [3] to compute sensitivities without analytical adjoint formulations and a checkpointing algorithm to reduce the memory requirements for storing information from implicit iterations. We formulate an optimization problem in terms of the drag force of dispersed particle flow and demonstrate the efficacy of the proposed method through some numerical examples.

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THE C-N FATIGUE LAW FOR EVALUATING THE CYCLE-LIFE OF LITHIUM-ION BATTERIES

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ABSTRACT

Fatigue in LIBs is process-sensitive: variation in (dis)charging profiles and operating temperatures are known to be responsible for differences in cycle-life. Furthermore, when the same batch of batteries is tested under the same environmental conditions, their cycle-life scatters. Scattering cycle-life of LIBs further complicates lifetime prediction for LIBs, which is pivotal to engineering practice since batteries are often used in packs and modules. The dependence of critical fatigue parameters on ambient temperature and charging or discharging rate, along with the scattering nature of LIBs' cycle-life remains unknown, which desires novel theoretical innovations.

Through large-scale experimental investigations and systematic data mining, we demonstrated that the charging rate C and the resulted cycle-life N of batteries obey C= c_0*N^b, named as C-N fatigue depedence. In this equation, c_0 is a limiting charging rate that is the minimum charging rate causing battery failure during the first cycle, and b is battery-type related constant. In the log-log coordinate, the C-N curve exhibit a linear dependence, in which c_0 is the intercept and b is the slope. By investigating the C-N fatigue dependence at various discharging rates and fixed temperature, it is further indicated that b is a function of the discharging rate (D) and c_0 is irrelevant to D. In parallel, the authors decipher the effect of temperature upon cycle-life properties of batteries. It is found that the power b of the C-N curve is insensitive to variation in temperature. The limiting charging rate c_0, in contrast, shows strong dependence on ambient temperature. In combination, the C-N fatigue depedence may be further refined as C=c_0(T)*N^b(D). Based on different statistical investigations, the group reveals that the lognormal distribution is the appropriate model for cycle-life scattering analyses of LIBs. For the first time, a probabilistic C-N (P-CN) model is derived for quantifying the fatigue failure probability in LIBs. The above achievements offer novel mechanical insights to analyzing the cycle-life performance, performing health management, and optimizing module designs for LIBs.

Advanced machine learning methods for multiscale modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADVANCING STABILITY IN DEEP LEARNING: EXPLORING THE SUPERIORITY OF SQRRESNET IN FUNCTION INTERPOLATION, COMPUTER GRAPHICS, AND PDE PROBLEM-SOLVING

C-S David Chen[*1], Amir Noorizadegan[1], Kenji Kawaguchi[2] and Der-Liang Young[1]*

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ABSTRACT

This study introduces an innovative strategy to enhance the stability of adaptive feedforward architectures in deep learning, specifically focusing on function interpolation, computer graphics, and partial differential equations (PDEs). The proposed approach leverages a distinctive Residual Network (ResNet) variant, the squared residual network (SqrResNet). While ResNet is commonly associated with convolutional neural networks, SqrResNet stands out as an excellent algorithm for integration into feedforward networks, substantially improving computational stability. The investigation thoroughly explores back-propagated gradients to loss values, underscoring SqrResNet's exceptional ability to balance different loss terms during model training. This represents a clear improvement over plain neural networks and ResNet. In the domain of function interpolation, we evaluate both smooth and non-smooth functions in both 2D and 3D settings. Furthermore, SqrResNet is tested in computer graphics scenarios involving intricate models such as the Stanford Bunny and in medical imaging applications. The method extends to solving forward and inverse PDE problems, with a detailed comparison to the DeepXDE package using a plain neural network in its feedforward algorithm. The following observations have been made across various examples in these diverse fields:

- SqrResNet consistently outperforms both ResNet and plain neural networks, demonstrating superior accuracy, stability, and convergence.
- SqrResNet stands out for its impressive performance, especially when plain neural networks struggle to train or face divergence shortly after some epochs.
- SqrResNet exhibits exceptional stability, even with over 50 hidden layers, aiming for enhanced accuracy.
- The study underscores the problem-dependent nature of the number of hidden layers, revealing that deeper networks (exceeding ten hidden layers) often yield better accuracy. In contrast, plain neural networks opt for fewer hidden layers to address instability with larger layer counts.

These findings underscore the substantial advantages of SqrResNet over conventional ResNet and plain neural network architectures.

Transport phenomena in micro/nanofluids
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SINGLE-PARTICLE DYNAMICS IN A LOW-REYNOLDS-NUMBER FLUID UNDER SPHERICAL CONFINEMENT

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ABSTRACT

Non-colloidal dynamics of a single particle suspended in a low-Reynolds-number fluid under spherical confinement was studied numerically. We calculated hydrodynamic mobilities of a sphere, a prolate spheroid and an oblate spheroid parallel and transverse to the particle-cavity line of centres. The mobilities show maximum in the cavity centre and decay as the particle moves towards the no-slip wall. For prolate and oblate spheroids, their mobilities are also affected by the angle between the particle's axis of revolution and the particle-cavity line of centres due to particle anisotropy. It was observed that the effect of particle anisotropy becomes stronger as the confinement level increases. When the external force on the particle is not parallel or transverse to the particle-cavity line of centres, a drift velocity perpendicular to the force occurs because of the confinement-induced anisotropy of the mobility in the cavity. The normalized drift velocity depends on the particle location, size, shape and orientation of the non-spherical particle. We also studied the motion of a non-neutrally buoyant particle under external forces in a rotating flow inside the cavity. Cooperation between the external force, rotation-induced centrifugal or centripetal force and the force from particle–wall interactions leads to multiple modes of particle motion. A fundamental understanding of single-particle dynamics in this work forms the basis for studying more complex particle dynamics in intracellular transport, and can guide particle manipulation in microfluidic applications ranging from droplet-based microreactors to microfluidic encapsulation.

Fluid-structure interaction in interface and moving boundary problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A PARTITIONED COUPLING ALGORITHM FOR HIGH-FIDELITY HYDRODYNAMIC INDUCED STRUCTURAL FRACTURE ANALYSIS

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ABSTRACT

The main focus of this work is to develop a partitioned coupling algorithm for high-fidelity structural fracture simulations subjected to hydrodynamic impacts. This is achieved by combining the finite volume method (FVM) with an intrinsic cohesive zone model (CZM). Fluid flows are simulated with the aid of the FVM in conjunction with the volume of fluid method to resolve the two-phase interface. Moving meshes are effectively managed using the arbitrary Lagrangian-Eulerian method. Our algorithm describes crack onset and propagation using the CZM in the context of finite element modeling. The partitioned strategy to couple the fluid and structure domains is implemented by recourse to a multi-physics open-source coupling library, i.e., preCICE. Mesh types and connectivity of both fluid and structure parts are incorporated into solver adapters, facilitating data exchange and mapping between non-matching meshes. We introduce a parallel implicit scheme to enhance coupling convergence, complemented by a Quasi-Newton scheme to stabilize and accelerate the fixed-point iteration at the coupling interface. Additionally, a second-order precision nearest-projection mapping method is employed for data mapping between non-matching meshes on the coupling interface. The coupling algorithm facilitates efficient parallel computation in High-Performance Computing clusters. The communication channel is established through TCP/IP sockets, and the infiniband system serves as the network interface for data communication among multiple computational hosts. Several representative numerical examples are performed to demonstrate the accuracy, efficiency, and effectiveness of our presented coupling algorithm.

Computational particle-based solvers for multiphysics & multiscale simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADVANCING MULTI-SCALE PHYSICS MODELING IN STRONGLY MAGNETIZED RELATIVISTIC PLASMAS: AN ANALYTICAL PARTICLE PUSHER APPROACH

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ABSTRACT

Originally developed by F.H. Harlow at LANL for hydrodynamic simulations, Particle-in-Cell (PIC) methods are now widely employed in simulating fluid and kinetic plasmas across diverse application domains, including fusion studies, plasma-based accelerators, space, and laboratory plasmas. However, addressing multi-scale physics in astrophysical and laboratory plasmas with strong magnetic fields poses challenges for conventional PIC methods. This has important consequences for understanding particle acceleration and emission mechanisms for a wide range of laboratory and astrophysical systems.

In this study, we leverage a known analytical solution for particle motion in arbitrary constant electromagnetic fields [1,2] to develop approximate solutions with non-uniform fields. This novel approach allows for significant improvements in simulation accuracies and achievable scales within the kinetic model when strong magnetic fields are present, which are unattainable with standard methods. We will showcase the advantages of the analytical particle pusher and the resulting PIC algorithm compared to conventional approaches, demonstrating its efficacy through standard test-particle and self-consistent benchmarks.

Furthermore, we will conduct a thorough comparison between the new algorithm and standard PIC methods in more realistic scenarios, such as relativistic shocks, covering regimes from relatively weak to strong magnetizations. This study aims to shed light on the enhanced capabilities of the proposed analytical particle pusher and its potential impact on advancing our understanding of plasma dynamics in multi-scale astrophysical environments.

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Uncertainty quantification and reliability analysis in engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DIRECT PROBABILITY INTEGRAL METHOD FOR HIGH-DIMENSIONAL STOCHASTIC MECHNICAS ANALYSIS

Guohai Chen[*1] and Dixiong Yang*[1]

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ABSTRACT

Engineering structure is a complex system with a large number of degrees of freedom. Due to suffering from various uncertainties during the construction and service life cycle, the randomness involved in structural parameters and environmental loads forms a high-dimensional input probability space, which makes the uncertainty propagation of the structural system from input to output being a challenging issue. The dimension reduction is a conventional approach to solve this issue, but it also makes the essential characteristics of system difficult to be truly reflected. Monte Carlo simulation (MCS) seems to be dimension-independent, but it needs a large number of samplings. To this end, based on the principle of conservation of probability, this study derives the basic equation governing the propagation of probability density from input to output in the time-space domains, named as probability density integral equation (PDIE). By combining structural equilibrium equation and PDIE, the direct probability integral method (DPIM) is proposed to perform stochastic response and reliability analyses of linear/nonlinear, time-independent/time-dependent structures in a unified way. In this framework, the structural equilibrium equation can be solved by analytical or numerical methods, and the partition of probability space and smoothing technique of Dirac delta function are presented to solve PDIE numerically, to achieve the probability density function of the structural responses. From the perspective of PDIE, this study reveals the relationship between DPIM and MCS, and why MCS is dimension-independent but requires a huge amount of computation. Furthermore, a new probability space partitioning strategy is proposed for the high dimensional probability space, and DPIM is extended to high dimensional stochastic mechanics. The new probability space partition strategy does not need to reduce the dimension of structural system, and the computational cost is greatly reduced. Finally, the numerical examples demonstrate the effectiveness and applicability of DPIM in high-dimensional stochastic mechanics.

Multi-scale and machine learning-based modeling methods for optimization and design of composites
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL SIMULATION ON THE STRESS RUPTURE LIFE OF 2D-C/SIC UNDER HIGH TEMPERATURE AND WET OXYGEN CONDITION

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ABSTRACT

C/SiC composites with high specific strength/stiffness are important candidates for thermal structures of new-generation hypersonic aircraft, and the main failure mode of this material is stress-oxidation failure under high temperature and wet-oxygen service environments. To further understand the performance of this material under high-temperature and wet-oxygen service conditions, this study takes C/SiC composites as the research object and establishes a multi-physical-field coupled high-temperature stress oxidation model in combination with numerical simulation to carry out the stress oxidation life study.

This study first established a diffusion coefficient equation based on the oxidation law of the carbon phase in a wet oxygen environment. It then mapped the relationship between external load, environmental conditions, and oxidation, and established a comprehensive failure criterion for stress oxidation under a high-temperature wet oxygen environment. Next, we introduce the criterion of overall failure due to stress oxidation into the finite element model of C/SiC composite material. We write a VUMAT user subroutine and simulate the progressive failure process of the composite material by adopting the method of element failure, and achieve the simulation of stress oxidation life. Finally, to carry out the numerical simulation study of the stress oxidation life of C/SiC composites, verify the accuracy of the model by testing data, and analyze the effect of temperature and external load on the stress oxidation life.

Research results show that at 1300℃, the stress oxidation life with the increasing of external load shows a decreasing trend, which roughly shows an exponential function trend; at 140MPa external load, the stress oxidation life with the increasing of temperature appears to decrease firstly, and then increase with the increasing of temperature, which shows a generally parabolic trend.
In this study, we established a multi-physics field coupling high-temperature stress oxidation numerical simulation method through the numerical simulation study of high-temperature stress oxidation of C/SiC composites and obtained a more realistic numerical simulation model of high-temperature stress oxidation of C/SiC composites, which provides a technical basis for the assessment of the high-temperature service performance of C/SiC composites structures.

Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A GENERALIZED PERIDYNAMIC MATERIAL CORRESPONDENCE FORMULATION USING NON-SPHERICAL INFLUENCE FUNCTIONS

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ABSTRACT

Peridynamics theory is a nonlocal continuum mechanics theory. The peridynamic material correspondence formulation provides passage for direct incorporation of any constitutive models from the conventional local continuum mechanics theory. However, the conventional material correspondence formulation suffers from the well-known issue of material instability. The material instability in peridynamics can be understood as the existence of non-unique mapping between deformation states and the resultant force state. This instability poses practical difficulties while using the correspondence model in computational modeling. One consequence of this instability is the oscillation in the predicted displacement field, i.e., existence of zero-energy modes.

Research efforts have been devoted to remedy the material instability issue, such as introducing additional stabilizing force term and formulating bond-associated deformation gradient using a subset of the horizon. In this presentation, a new class of influence functions is proposed to inherently remove the material instability in the material correspondence formulation. The currently used influence function in the literature is spherical and depends only on the scalar state of a bond. A new class of bond-associated influence functions that depend on the bond length and angle between bonds will be introduced. New material correspondence formulation is developed based on the bond-associated influence function. Numerical examples including influence function analysis, wave dispersion analysis, and deformation prediction are studied to test the validity and effectiveness of the developed model. Conclusion and future work are discussed.

Uncertainty quantification and reliability analysis in engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STOCHASTIC RESPONSE CHARACTERISTIC ANALYSIS OF UNDERWATER STRUCTURE BASED ON HYBRID DPIM–SBM

Hanshu Chen[*1], Guohai Chen[2], Dixiong Yang[2] and Zhuojia Fu[1]*

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ABSTRACT

The ocean is an abundant source of valuable resources for humanity. As the exploitation of these resources increases, so does the use of underwater vehicles for exploration activities. However, the unpredictable nature of the ocean environment poses significant challenges to the operation and trajectory planning of underwater vehicles. Therefore, accurately predicting the stochastic response characteristics of underwater vehicles in random ocean environments is of utmost importance. This study focuses on a novel type of underwater vehicle equipped with a rudderless paddle. Adopting this vehicle as the research subject, the probability density integration equation (PDIE) of the system is derived based on the principle of probability conservation. Furthermore, a direct probability integration method (DPIM) based on block parallel computing is proposed. This method effectively decouples the control equations of the underwater vehicle system from PDIE and utilizes block-parallel computation techniques, enabling efficient stochastic response analysis of the new underwater vehicle under random wave excitation. The results indicate that the significant height of sea waves and flow velocity are the primary stochastic factors affecting the response of underwater vehicles. Higher significant wave heights and flow velocities increase the probability of deviation from the predetermined trajectory of underwater vehicles and may lead to random jumping phenomena, thereby reducing the navigation safety of underwater vehicles.

Advanced materials: Computational analysis of properties and performance
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TEMPERATURE AND COMPOSITION DEPENDENT CRITICAL RESOLVED SHEAR STRESS OF BASAL SLIP IN MG-Y ALLOY FROM LARGE-SCALE MOLECULAR DYNAMICS

Huicong Chen[*1] and Jun Song[1]*

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ABSTRACT

Magnesium (Mg) has attracted significant interest in the manufacturing and transportation sectors due to its low density, abundance in the earth's crust, high specific strength, and good castability. However, Mg and its alloys typically exhibit poor room temperature ductility and formability, which limits their use as wrought materials. These limitations are directly linked to the underlying hexagonal-close-packed (hcp) crystal structure, which lacks sufficient independent deformation modes for homogeneous deformation at low temperatures. Increased ductility of magnesium is achieved via alloying with certain solutes, which can change activation of different slip systems due to solute strengthening.

This study investigates the impact of solute atoms (Y) on the critical resolved shear stress (CRSS) for basal slip in Mg alloys across a wide range of temperatures and solute contents. Molecular dynamics simulations were extensively employed to determine the influence of Y on CRSS, while kinetic Monte Carlo simulations were used to examine solute segregation at dislocation cores. In random solid solutions, the presence of solute–dislocation and solute–solute interactions led to a monotonic increase in CRSS with increasing Y concentration, even at elevated temperatures. Furthermore, Monte Carlo simulations revealed that Y atoms exhibited segregation tendencies at dislocation cores. Subsequent molecular dynamics simulations demonstrated that such segregation exerted a stronger pinning effect on the motion of dislocation. The current simulation shows a promising pathway of improvement for ductility of Mg alloys by controlling the content of Y at finite temperature.

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A FULLY COUPLED CELLULAR AUTOMATON-MATERIAL POINT METHOD FOR SOLIDIFICATION GRAIN STRUCTURE PREDICTION DURING THE METAL ADDITIVE MANUFACTURING PROCESS

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ABSTRACT

In this study, we proposed a fully coupled three-dimensional cellular automaton-material point method (fc-CAMPM) for simulating the material deposition and microstructure evolution in metal additive manufacturing (AM). In this method, the multi-physics material point method (MPM) is utilized to solve the thermo-fluid-solid coupling problem at the powder scale. The MPM for the temperature field is fully coupled with the 3D cellular automaton (CA) for the solidification microstructures evolution. In the fully coupled framework, the fraction of solid can be timely calculated for each MPM cell based on the solidification front of the microstructure to update the temperature field. with an accurate latent heat release or absorption. In return, the MPM can provide a more realistic solidification path for the CA. Due to significant differences in cell sizes and time steps between MPM and CA, we proposed a dynamic cell activation technique to reduce the computational cost during fully coupled solving. In this technique, only CA cells within the mushy zone are activated for grain nucleation/growth simulation in each step of CA, while the information of other solid cells is stored in memory. Several numerical examples are presented to showcase the effective and efficiency of the proposed method. It is demonstrated that the fc-CAMPM is a powerful tool for revealing the microstructure evolution mechanism and further to advance the understanding of the microstructure-property relationship during the metal AM.

Data-driven approaches for solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

N-ADAPTIVE RITZ METHOD: A NEURAL NETWORK ENHANCED COMPUTATIONAL MECHANICS FRAMEWORK

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ABSTRACT

Conventional finite element methods are known to be tedious in adaptive refinements due to their conformal regularity requirements. Meshfree methods, such as the Reproducing Kernel Particle Method, relaxed the discretization and approximation regularity requirements in finite elements, however the enrichment functions for adaptive refinements are not readily available in general applications. The fast-growing research and development in data science, machine learning and artificial intelligence offer new opportunities for the development of new paradigms in scientific computing. This talk presents a neural network (NN) enhancement of Galerkin solution for weak and strong discontinuities, as well as for solution enhancement with a fixed discretization, called N-adaptivity. The flexibility and adaptivity of the NN function space are utilized to capture complex solution patterns that the conventional Galerkin methods fail to capture. The NN enrichment is constructed by combining pre-trained NN blocks with an additional untrained NN block. The pre-trained NN blocks learn specific complex solution patterns during the offline stage, enabling efficient enrichment of the approximation space during the online stage through the Ritz-type energy minimization. The NN enrichment is introduced under the Partition of Unity (PU) framework, ensuring convergence of the proposed method.

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Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THERMODYNAMICS-BASED DATA-DRIVEN COMPUTING FOR INELASTIC MATERIALS MODELING

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ABSTRACT

Characterization and modeling of complex materials by phenomenological models remains challenging due to difficulties in formulating mathematical expressions and internal state variables (ISVs) governing path-dependent behaviors. Data-driven machine learning models, such as deep neural networks and recurrent neural networks (RNNs), have become viable alternatives. However, pure black-box data-driven models mapping inputs to outputs without considering the underlying physics suffer from unstable and inaccurate generalization performance. This study introduces a machine-learned physics-informed data-driven constitutive modeling approach for path-dependent materials based on the measurable material states. The proposed data-driven constitutive model is designed with the consideration of universal thermodynamics principles, where the ISVs essential to the material path-dependency are inferred automatically from the hidden state of RNNs [1]. For materials subjected to fracturing or strain localization, a neural network enriched Galerkin solution for weak and strong discontinuities and for adaptive refinement without re-meshing is introduced [2, 3]. Applications to plasticity, localization and fracture modeling using the proposed methods will be presented.

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Multi-physics and multi-scale simulations with the coupling library preCICE
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SPEED UP THE MULTI-SCALE SIMULATIONS WITH PRECICE AND MICROMANAGER: RESULTS PRESENTED FOR A POROUS-MEDIA FLOW

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ABSTRACT

We aim to increase the computational efficiency of the multi-scale simulation of a flow-field in porous media. There, the macro-scale solver is provided with real-time local properties up-scaled from the outcome of micro-scale simulations. This up-scaling is proven to be superior to resorting to standard empirical equations for the local field description, especially in more complex scenarios like multi-phase flow, with the cost of much more computing time. A general framework to lower the cost is needed.

We partition the simulation into unit solvers for different scales and use the preCICE library to couple them together. Thus, we can focus on improving the general coupling method without touching the case-specific unit solvers.

We also employ the Micro Manager extension in preCICE as a wrapper for all micro simulations and to use its adaptivity features, with which Micro Manager completes the large amount of micro-scale simulations efficiently by solving a couple of representative points and reusing these results to all the other points with adequate similarity.

We contribute to Micro Manager by enabling the adjustment of the strictness of the similarity evaluation based on the current convergence status. It helps to get rid of unnecessarily accurate results at the early stage of the simulation but also brings in the challenge of balancing between solving fewer micro-scale points and retaining the convergence property of the coupled simulation.
We are also working on improving the existing Quasi-Newton(QN) methods in preCICE, which expedites convergence, to handle physical values within specific ranges, e.g. to avoid negative density or phase concentration etc. This would benefit all the simulations, where bounded values are involved in the QN methods.

The performance of the dynamic similarity condition and the QN methods for bounded values will be shown with the results of the two-scale simulation of a multi-phase porous media flow, in which the unit solvers in both scales are implemented in DuMuX. While we treat the unit solvers as black-box in preCICE and MicroManager, the same method would be helpful for other multi-scale simulations coupled with them.

Advanced materials and smart structures: Modeling, simulation and testing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

METASTRUCTURES WITH SHUNTED PIEZOELECTRIC PATCHES

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ABSTRACT

Low-frequency noise and vibration suppression have long been research sujects over decades. Phononic crystals (PCs) poessessing Bragg scattering mechanism can create bandgaps over certain frequency range. Due to the structure size limit, those crystals are ineffective in the low frequency regime. The emergence of locally resonant (LR) acoustic/elastic metamaterials has provided an additional avenue for eliminating unwanted noise/vibration. Those structures exhibits the phenomenon of LR bandgaps, which is useful for manipulating wave propagation. The local resonating units include spring-mass, cut-out, beam-like, force-moment, cantilever-mass, pillar-type structures, and etc. The bandgap properties can be determined by the geometry of the resonating unit cell. Membrane-type metamaterials have also been considered as potential LR systems. Changing their physical properties, such as membrane tension and mass weight, can tailor bandgap location. However, the the durability issue of membrane tension still remains challenging. Recently, the use of piezoelectric materials has demonstrated their effectiveness in enriching the dynamic characteristics of LR bandgaps. By adjusting the parameters of shuting circuit, the bandgap frequencies can be easily tuned. In this study, two metastructures integrated with shunted piezoelectric circuits are proposed. One is comprised of an elastic base beam with array-type sub-beam structtures; the other is an ealstic plate with shunted piezoelctric films. Theoretical models and finite element analysis are used to predict the vibration transmission. The effects of circuital parameters on attenuation constants are investigated. Multi-frequency wave attenuation can be achieved by adding extra shunted patches. The proposed tunable metastructures might boost the development of vibration control devices.

Computational mechanobiology of musculoskeletal tissues
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RE-ORIENTATION OVER RE-ALIGNMENT: ULTRASTRUCTURAL RESPONSES OF CARTILAGE COLLAGEN FIBRILS TO MECHANICAL LOADING

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ABSTRACT

Articular cartilage is renowned for its crucial mechanical roles in load bearing and shock absorption, effectively distributing load and safeguarding the subchondral bone. Its biomechanical properties arise from its extracellular matrix (ECM), comprising a collagenous network interacting with proteoglycan-rich interstitial fluid. The collagen fibrils in the cartilage exhibit depth-dependent organisation, forming three distinct zones—superficial, transitional, and deep—each responding uniquely to external loads. Maintaining these depth-dependent characteristics is essential for the cartilage's biomechanical functionality. The deterioration of these structural traits is linked to cartilage lesions and degenerative disorders like osteoarthritis (OA). Significant research endeavours aim to quantitatively correlate cartilage structure with its biomechanical efficacy, a challenge compounded by collagen's complex hierarchical organisation and the collective responses of the zonal structures to mechanical loading.

Recent advancements in polarisation-resolved second harmonic generation (pSHG) microscopy [1] have enabled probing of collagen organisation beyond optical resolution in a label-free, depth-sectioning manner. This technique has unveiled the hierarchical complexity of fibrillar organisation at nanometre scales and intrafibrillar organisation at the molecular level in cartilage [2]. These findings are critical in understanding local ECM behaviours and their role in mechanotransduction to embedded chondrocytes, thus influencing cartilage synthesis and homeostasis. The rapid scanning capability of pSHG facilitates visualisation of dynamic structural responses to mechanical or chemical stimuli, with collagen organisation at both length scales showing marked sensitivity.

Our study primarily aims to visualise and quantify the spatial gradient and heterogeneity of collagen organisation in bone-cartilage explants, focusing on the principal orientation and degree of alignment at the ultrastructural level. We examine the mechanical responses of this gradient ultrastructure to external loads at various strain intervals. This involves assessing the re-orientation and re-alignment of collagen fibrils to understand the collective role of cartilage zonal organisation in dictating the tissue's overall mechanical behaviour. Utilising pSHG, we captured collagen organisation across the longitudinal plane of cartilage-bone explants with high spatial resolution. A customised loading rig, integrated with our multiphoton platform, enabled loading to the tissue during imaging acquisition. Our findings indicate that the transitional zone undergoes the most significant changes in response to mechanical loading, primarily through collagen fibre re-orientation rather than re-alignment.

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Data-driven methods for modeling complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PSEUDO-DIFFERENTIAL INTEGRAL AUTOENCODER NETWORK FOR INVERSE PDE OPERATORS

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ABSTRACT

Partial differential equations (PDEs) play a foundational role in modeling physical phenomena. This study addresses the challenging task of determining variable coefficients within PDEs from measurement data. We introduce a novel neural network, "pseudo-differential IAEnet" (pd-IAEnet), which draws inspiration from pseudo-differential operators. pd-IAEnet achieves significantly enhanced computational speed and accuracy with fewer parameters compared to conventional models. Extensive benchmark evaluations are conducted across a range of inverse problems, including Electrical Impedance Tomography (EIT), optical tomography, and seismic imaging, consistently demonstrating pd-IAEnet's superior accuracy. Notably, pd-IAEnet exhibits robustness in the presence of measurement noise, a critical characteristic for real-world applications. An exceptional feature is its discretization invariance, enabling effective training on data from diverse discretization schemes while maintaining accuracy on different meshes. In summary, pd-IAEnet offers a potent and efficient solution for addressing inverse PDE problems, contributing to improved computational efficiency, robustness, and adaptability to a wide array of data sources.

The phase field method for fracture: Theory, numerics, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MIXED-MODE CRACK OPENING COMPUTATION IN THE PHASE FIELD METHOD

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ABSTRACT

The phase field modelling of cracks gains popularity in the fracturing analysis recently, due to its smeared representation of cracks, avoiding the introduction of geometric discontinuities and remeshing around crack tips. The method has been cast in both brittle and cohesive format. In the analysis, the crack opening displacement is an essential variable for the cohesive fracture model, due to the dependence of the fracture energy on it. For the brittle fracture model, the crack opening displacement is also crucial in certain applications, e.g., hydraulic fracturing or fracturing in the oil and gas exploration. In the current study, the full form of the mixed-mode crack opening is derived for the first time in the framework of phase field modelling. The formulations are given separately for the brittle and cohesive fracture model. The crack opening displacement is associated with a line integral normal to the crack. Different factors and matrices apply in the integration for both fracture models and crack directions. The derivations are validated analytically by an edge cracked problem and numerically by curved crack issues.

DERIVATIVE-INFORMED DEEPONETS FOR HIGH-DIMENSIONAL PARAMETRIC PDES

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ABSTRACT

Deep operator networks (DeepONets), a class of neural operators that learn mappings between function spaces, have recently been developed as surrogate models for high-dimensional parametric partial differential equations (PDEs). In this talk, we introduce a derivative-informed deep operator network (DI-DeepONet), which leverages the derivative information of the solution operator of parametric PDEs to enhance the accuracy and efficiency of DeepONet. DI-DeepONet uses DeepONet as its backbone and incorporates two derivatives in the loss function for training, including the directional derivatives of the output function with respect to the input function and the gradient of the output function with respect to the physical domain variables. This feature enhances generalization accuracy, especially in scenarios with limited training data, and provides a more accurate approximation of derivatives. Additionally, we propose to use a reduced representation of the input functions (e.g., through projection into the Karhunen–Loève expansion subspace or the active subspace) rather than the full representation. The model-based dimension reduction of input functions allows us to train a much smaller neural network, thereby significantly reducing the computational cost for training and the required volume of training data. We present the results of several numerical experiments to demonstrate the effectiveness of DI-DeepONet compared to DeepONet.

Machine learning for large scale models in physics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CROM: CONTINUOUS REDUCED-ORDER MODELING OF PDES USING IMPLICIT NEURAL REPRESENTATIONS

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ABSTRACT

The long runtime of high-fidelity partial differential equation (PDE) solvers makes them unsuitable for time-critical applications. We propose to accelerate PDE solvers using reduced-order modeling (ROM). Whereas prior ROM approaches reduce the dimensionality of discretized vector fields, our continuous reduced-order modeling (CROM) approach builds a low-dimensional embedding of the continuous vector fields themselves, not their discretization. We represent this reduced manifold using continuously differentiable neural fields, which may train on any and all available numerical solutions of the continuous system, even when they are obtained using diverse methods or discretizations. We validate our approach on an extensive range of PDEs with training data from voxel grids, meshes, and point clouds. Compared to prior discretization-dependent ROM methods, such as linear subspace proper orthogonal decomposition (POD) and nonlinear manifold neural-network-based autoencoders, CROM features higher accuracy, lower memory consumption, dynamically adaptive resolutions, and applicability to any discretization. For equal latent space dimension, CROM exhibits 79X and 49X better accuracy, and 39X and 132X smaller memory footprint, than POD and autoencoder methods, respectively. Experiments demonstrate 109X and 89X wall-clock speedups over unreduced models on CPUs and GPUs, respectively. Videos and codes are available on the project page: https://crom-pde.github.io.

SciML in the real world
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LEARNING NEURAL CONSTITUTIVE LAWS FROM MOTION OBSERVATIONS FOR GENERALIZABLE PDE DYNAMICS

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ABSTRACT

We propose a hybrid neural network (NN) and PDE approach for learning generalizable PDE dynamics from motion observations. Many NN approaches learn an end-to-end model that implicitly models both the governing PDE and constitutive models (or material models). Without explicit PDE knowledge, these approaches cannot guarantee physical correctness and have limited generalizability. We argue that the governing PDEs are often well-known and should be explicitly enforced rather than learned. Instead, constitutive models are particularly suitable for learning due to their data-fitting nature. To this end, we introduce a new framework termed “Neural Constitutive Laws” (NCLaw), which utilizes a network architecture that strictly guarantees standard constitutive priors, including rotation equivariance and undeformed state equilibrium. We embed this network inside a differentiable simulation and train the model by minimizing a loss function based on the difference between the simulation and the motion observation. We validate NCLaw on various large-deformation dynamical systems, ranging from solids to fluids. After training on a single motion trajectory, our method generalizes to new geometries, initial/boundary conditions, temporal ranges, and even multi-physics systems. On these extremely out-of-distribution generalization tasks, NCLaw is orders-of-magnitude more accurate than previous NN approaches. Real-world experiments demonstrate our method’s ability to learn constitutive laws from videos.

Multiscale, multifield, and continuum-discontinuum analysis in geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A SET OF HYSTERETIC NONLINEAR CONTACT MODELS FOR DEM AND APPLICATION FOR DEFORMABLE GRANULAR PARTICLE FLOW

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ABSTRACT

In the discrete element method (DEM), contact models describe how particles interact with each other and with boundaries, and are a key element to capture the bulk behavior of a granular system. In this work, we propose a set of hysteretic nonlinear contact models for approximating the bulk strain-hardening phenomena of relatively soft granular materials. These contact models comprise simple polynomial and/or exponential functions to allow for easy calibration. To ensure numerical stability, we have derived unconditionally stabilized viscous damping force models. The resultant DEM model is implemented in LIGGGHTS-INL and applied to simulate an axial compressibility test and hopper flow for deformable granular materials. Results show that the DEM model can reproduce the bulk stress–strain profiles of the physical samples and that the predicted responses agree reasonably with the experimental data.

Modeling friction and wear
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE STEADY STATE OF THE OSCILLATORY ADHESIVE CONTACT BETWEEN A RIGID CONE AND A VISCOELASTIC HALF-SPACE

Shiwen Chen[*1], Xuan-Ming Liang[1] and Gangfeng Wang[1]*

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ABSTRACT

The steady-state responses in the oscillatory indentation test are widely adopted to evaluate the viscoelastic behavior of cells and tissues. In such tests, the strong adhesion of biomaterials is, however, commonly neglected due to the difficulty in solving the coupled adhesive viscoelastic contact problems. In our research, by introducing the interfacial interaction described by Lennard-Jones potential using connector elements, we develop a finite element method to simulate the oscillatory adhesive contact between a rigid cone and a viscoelastic half-space. It is shown that with a sinusoidal displacement excitation, the reaction force evolves sinusoidally at the same frequency but they are not perfectly in phase. The interfacial adhesion will magnify the amplitude of force vibration while weaken the average strength. For weak adhesion, the mean contact force shows little dependence on the excitation frequency, whereas for strong adhesion, the dependence becomes apparent. The phase difference between the reaction force and the displacement excitation could be either aggravated or eased depending on the strength of adhesion. It is observed that the phase difference attains its maximum at an intermediate strength of adhesion, and approaches the argument of the complex modulus of the viscoelastic substrate as the strength of adhesion increases. The present study can provide guidance for the development of the oscillatory indentation test on viscoelastic materials.

Recent advances in computational fracture mechanics and failure analysis
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LAGRANGE MULTIPLIER/COHESIVE ZONE (LM/CZ) METHODS FOR MULTIPLE CRACK SIMULATIONS

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ABSTRACT

Currently, accurate simulations of cracks remain a challenging task in computational mechanics community. In light of this, we have developed a series of nodal-based Lagrange multiplier/cohesive zone (LM/CZ) methods for accurate crack simulations. We consider two different crack patterns, i.e., those crack paths are known and unknown in prior. Special focus is given to the interactions between different crack patterns. The developed methods are capable of dealing interface cracks with matching and non-matching meshes. The main idea of the presented methods is to fulfil the displacement compatibility condition at finite element nodes before crack onset via LMs. The LM forces at each nodal pair are calculated in a predictor-corrector form with a limited number of iterations. The nodal constraints are smoothly switched to cohesive forces after a defined criterion is satisfied. Compared with the conventional intrinsic CZMs, our developed methods can effectively address the so-called artificial compliance numerical issue, thereby yielding more accurate numerical results. Several benchmark numerical examples are performed to demonstrate the numerical accuracy and effectiveness of our developed methods.

Physical models and reduced order models augmentation with data for physics-informed machine learning in real-world applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

REAL-TIME OPTIMISATION OF COMPOSITES FORMING PROCESS

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ABSTRACT

In the context of Industry 4.0, the aerospace and composites sectors are increasingly focusing on digitalised manufacturing techniques. With advancements in precise physically based computer modelling and machine learning algorithms, engineers are striving to actualise real-time optimisation and digital twin technologies. This framework promises the capability to adjust system parameters dynamically to achieve optimal or near-optimal performance based on virtual replicas of the physical manufacturing process, even under fluctuating conditions. These technologies significantly reduce trial-and-error costs, mitigating risks to the actual system, curtailing waste of expensive materials and energy, and saving the labour cost.

In liquid composites moulding, forming dry fibrous precursor materials into the mould's 3D shape before resin injection poses challenges, notably the high level of variability. This can lead to significant fabric defects such as out-of-plane wrinkles and folds that result is design tolerances not being met. Traditionally, composites weight saving advantages are not used to their full as “overdesign” is required to compensate for defect occurrence and a lack of process robustness. Finite element (FE) simulation tools, specifically developed for dry textile forming, can predict wrinkle formation under ideal conditions with good accuracy. However, uncertainties inherent to the process make the use of deterministic simulations almost useless and the extensive computational requirements of FE limit the number of simulations that can be run. This introduces difficulties for process parameter optimisation using traditional approaches.

This study introduces a real-time optimisation framework for dry fabric forming process. The framework is underpinned by a Gaussian process (GP) emulator trained on a small dataset built from FE simulations. Utilising dimension reduction and active learning algorithms, the GP emulator can explore a vast design space of control parameters without prior expert knowledge. The parameter range is then refined and an approximate optimal condition is found from running only a few hundred FE simulations. The trained emulator can predict real-time optimum conditions, given the measured fiber-direction variability as an input parameter. To validate the capability of the algorithms on a real-world system, a forming cell equipped with a multi-camera digital image correlation (DIC) system is built. This allows to measure the necessary preform variabilities, adjusts control parameters, and reconstructs the 3D mesh of the formed fabric's surface that can be compared with the simulation predictions. This research highlights the potential of data-driven digital twins in composite manufacturing, showcasing how the GP emulator can drive a digital twin with strong efficiency and accuracy.

Emerging topology and shape optimization techniques in computational design of materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DIFFERENTIABLE INVERSE DESIGN OF ACTIVE MORPHING MATERIAL SYSTEMS WITH MULTI-STIMULI RESPONSIVENESS

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ABSTRACT

Morphing material systems can alter shapes in response to stimuli, such as heat, light, or pH. This responsive morphing behavior provides exceptional controllability and adaptability to the system's functionality, enabling it to perform diverse tasks in varying environments. While this emerging materials paradigm holds significant promise in fields like soft robotics, minimally invasive surgery, and flexible electronics, existing studies predominantly concentrate on the manufacturing and modeling of responsive materials. There is a notable lack of an inverse design framework that can program a material system to achieve specific target shapes. While there are a few design-centric studies, they often focus on simple or periodic architectures, rely on heuristic optimizers, suffer from the computational burden of nested finite element analysis (FEA), overlook manufacturability, and are constrained to isotropic material responses and single stimuli.

In this study, we establish a proficient inverse design framework to tackle these challenges. This framework integrates differentiable simulation and extended topology optimization to program multi-stimuli shape morphing by co-designing the structure, stimuli, and manufacturing parameters. While the framework can accommodate various responsive materials, we focus on network systems made by 3D-printed liquid crystal elastomers (LCEs), which display anisotropic responsive behaviors, primarily contracting along the printing path when exposed to light or heat.

We first conduct experimental investigations into the constitutive and responsive behaviors of LCEs under varied printing speeds and pressures. Based on the results, we develop a differentiable simulation model that enables efficient GPU-backend simulations with auto-differentiation capability. We then extend topology optimization to accommodate mixed-variable design, concurrently optimizing the network system's nodal locations, connectivity, manufacturing parameters, and stimuli selection for each edge. This includes factors such as printing speed, pressure, and the number of layers, generating print-ready designs. We also incorporate manufacturing constraints into the design process to ensure printability. Built upon the automatic differentiation capability of our modeling, we can obtain the gradients of every design variable for all objectives, facilitating effective optimization without manual sensitivity derivation. Our method seamlessly integrates with a neural network-based objective function, allowing adaptation to arbitrary shape-morphing targets. The proposed methodology swiftly generates optimized network designs within minutes to program shape-morphing behaviors. It exhibits unparalleled flexibility in accommodating different network topologies, various initial and active shapes, and multiple stimuli, validated by both experiment and simulation. This inverse design framework can be generalized for use with other responsive materials, making it applicable to a range of robotic and surgical applications.

POTENTIAL THEORY METHOD FOR CONTACT PROBLEMS OF MATERIALS WITH MULTI-FIELD COUPLINGS

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ABSTRACT

We report a generalized potential theory method for the boundary-value problems of some advanced materials characterized by both anisotropy and multi-field coupling. The method is based on the original one proposed by Dr. Fabrikant, which is for transversely isotropic elastic materials. The generalization relies on the general solution established in the multi-field coupling cases. Different combinations of boundary conditions for multiple physical fields are considered. Exact, closed-form three-dimensional solutions are derived in terms of elementary functions are presented. Exact indentation relations are then established, which can be used in modern indentation techniques for characterizing material properties of advanced materials.

Data-driven modeling and design of materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GENERATIVE INVERSE DESIGN OF METAMATERIALS WITH FUNCTIONAL RESPONSES BY INTERPRETABLE LEARNING

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ABSTRACT

Metamaterials with functional responses, such as wave-based responses or deformation-induced property variation under external stimuli, can exhibit varying properties or functionalities under different conditions. Herein, we aim at rapid inverse design of these metamaterials to meet target qualitative functional behaviors. This inverse problem is challenging due to its intractability and the existence of non-unique solutions. Past works mainly focus on deep-learning-based methods that are data-demanding, require time-consuming training and hyperparameter tuning, and are non-interpretable. To overcome these limitations, we propose the Random-forest-based Interpretable Generative Inverse Design (RIGID), a single-shot inverse design method to achieve the fast generation of metamaterial designs with on-demand functional behaviors. Unlike most existing methods, by exploiting the interpretability of the random forest, we eliminate the need to train an inverse model mapping responses to designs. Based on the likelihood of target satisfaction derived from the trained forward model, one can sample design solutions using Markov chain Monte Carlo methods. The RIGID method therefore functions as a generative model that captures the conditional distribution of satisfying solutions given a design target. We demonstrate the effectiveness and efficiency of RIGID on both acoustic and optical metamaterial design problems where only small datasets (less than 250 training samples) are available. Synthetic design problems are created to further illustrate and validate the mechanism of likelihood estimation in RIGID. This work offers a new perspective on solving on-demand inverse design problems, showcasing the potential for incorporating interpretable machine learning into generative design and eliminating its large data requirement.

NUMERICAL STUDY ON THE BUBBLES BEHAVIORS ON COMPLEX GEOMETRIC SURFACES WITH COMPLEX WETTABILITY BASED ON 3D PHASE-FIELD LATTICE BOLTZMANN METHOD

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ABSTRACT

Bubbles trapped in the woven structures lead to the performance defects of composite materials. It is important to study the bubbles behaviors and regulation mechanism on the complex geometry and surface characteristics. A three-dimensional phase-field lattice Boltzmann method (PFLBM) for immiscible two-phase flow with large density and viscosity ratios was built, which takes into account surface tension, pressure force, viscous force and body force[1]. The three-phase wetting characteristics were successfully introduced on the plane and spherical surface by a geometrical way. The 3D two-phase model was validated by Laplace's law, and the wettability condition on the spherical surface was verified beacause the relative error between the measured and the specified contact angle is less than 2%. Then the complex geometric surfaces were constructed which consists of plane and spherical surface with complex wetting characteristics. An interpolation scheme was imposed at the junction lattices of two suface with differnet curvature. Basing on our built mathematical model, we systemly simulated a bubble motion on 3D complex geometric surfaces with complex wettability distribution. The geometrical shape, changable wettability, physical properties of fluids and driving force were investigated. By analyzing the force, flow field and shape evolution of the bubble in different moving stages, the bubble motion characteristics were got and the movement mechanism of the bubble on the complex geometric surfaces was revealed. Then we grasped how to control the bubble's behvaior on the complex surface shape with complex wettability distribution by surface tension, viscosity, driving force, wettability distribution, surface combined ways, surface curvature. The work would provide theoretical guidance and data support to improve the production quality of carbon fiber composites.
Key words: three-dimensional; phase-field lattice Boltzmann method; performance defects; complex geometric surfaces; wettability distribution

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Advanced computational mechanics based on data-driven techniques for structure, structural dynamics and aeroelasticity
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A COMPUTATIONAL FRAMEWORK FOR FRACTIONAL CONTRIBUTIONS FROM EXTERNAL LOADS TO THE FATIGUE OF LARGE-SCALE STRUCTURES

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ABSTRACT

Understanding the fractional contributions from external loads to the damage of complex engineering structures such as high-speed trains (HSTs) precisely is critical for their fatigue reliability design. We demonstrate in this paper a computational framework for identifying fractional contributions from wheel-rail excitations and aerodynamics to the fatigue of HST bogie frame based on multidisciplinary modeling. To this end, we first determine the stress at the vulnerable site for fatigue on the bogie frame of an HST subjected to aerodynamics and wheel-rail excitations under various conditions—single-train operation or two-train intersections in the open air or in the tunnel—using coupled aerodynamics, grid multi-body dynamics and structural finite element calculations. Then, we adopt the rainflow counting method to calculate the stress cycles and evaluate the structural fatigue life at the crucial site with the linear cumulative damage theory. Further, we develop metrics to quantify the individual and coupled contributions of each external load to the structural fatigue life. Moreover, in order to improve the efficiency of multidisciplinary calculations, we rely on machine learning models trained from very limited computational results to produce long-duration load data required for fatigue analysis. This paper clarifies the influence of different external loads on the fatigue of HST bogie frames under various working conditions. The findings may provide a foundation for designing fatigue-resistant critical structures of HSTs, and the developed framework may then supply a unified scheme for evaluating fractional contributions from external loads to the fatigue in many other large-scale structures.

Numerical modelling of composite materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NOVEL HIGH-ORDER SANDWICH PLATE THEORY-BASED ISOGEOMETRIC ANALYSIS FOR FREE VIBRATION OF VARIABLE ANGLE TOW COMPOSITE SANDWICH PLATES WITH COMPLEX-SHAPED CUTOUTS

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ABSTRACT

Advanced automated fibre placement technologies enable variable angle tow sandwich constructions possible, which provides an extended flexibility in stiffness tailoring to design lightweight sandwich plates with superior performance. However, complex-shaped openings within this new type of sandwich constructions bring great challenges when dealing with vibration problems. In this paper, an isogeometric analysis formulation based on a novel high-order sandwich plate theory is developed for the first time to the study of free vibration of variable stiffness sandwich plates with complex-shaped cutouts. The proposed new high-order sandwich plate model is formulated based on the idea of layerwise modeling, that is, the first-order shear deformation theory is applied to characterize the kinematics of the two skins, while the high-order theory based on hierarchic Legendre polynomials is utilized to describe the kinematics of the core. The weak-form governing equations associated with the vibration problem of the perforated sandwich plates is firstly derived from the virtual work principle, and then the IGA formulation based on the non-uniform rational B-splines (NURBS) is applied to obtain the eigenfrequencies and the corresponding vibration modes. The novelty of the current work lies in that the introduction of hierarchic Legendre polynomials enables the kinematics of the core to be enriched to any desired expansion order, and also brings some other merits such as the conciseness in derivation process and the easiness in program implementation, which shows great superiority over its traditional counterpart such as EHSAPT. On the other hand, the developed IGA procedure based on the novel high-order sandwich plate theory is applicable to a general sandwich plate even with complex-shaped cutouts. The accuracy and effectiveness of the developed IGA procedure are validated by comparing against the results available in literature and those obtained using ABAQUS. Effects of cutout size, boundary condition, and fiber angle on the vibration characteristics of the perforated sandwich plates are discussed in numerical examples. The results presented herein may be beneficial for the design of variable stiffness sandwich plates with complex-shaped cutouts.

Multiscale, multifield, and continuum-discontinuum analysis in geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DYNAMIC FRACTURE SIMULATION OF QUASI-BRITTLE MATERIALS USING A GENERALIZED MICROPOLAR PERIDYNAMIC MODEL

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ABSTRACT

A generalized micropolar micropolar peridynamic model is proposed to simulate the dynamic fracture behaviors of quasi-brittle materials. The governing equations of bonds connecting particles are reformulated from the definition of bond deformation rates, leading to a rate-based expression of mechanical behavior of solid particles. The peridynamic parameters are derived as time-dependent functions with the consistence of the strain energy obtained from the proposed peridynamic model and the continuum mechanics. The damage evolution functions are introduced in the model to capture the loading-rate dependence of rock. Moreover, a new failure criterion is proposed to describe the dynamic fracture progress of rock materials. The proposed model is verified by comparing its results with those from experimental observations. Numerical examples demonstrate that the dynamic fracture behaviors of rock materials under loads with different loading rates are well captured by the proposed model.

RESEARCH ON FIBER FRACTURE DAMAGE PATTERN RECOGNITION OF CMCS BASED ON DEEP FEATURES OF ACOUSTIC EMISSION SIGNAL

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ABSTRACT

Ceramic matrix composites (CMCs) are widely used in hypersonic vehicles and engines due to their excellent high-temperature mechanical properties. There are many types of microscopic damage mechanisms in the service process of CMCs, such as matrix cracking and fiber breakage, etc. Acoustic emission (AE) technology can monitor damage events online recognize the corresponding damage mechanism based on the AE signal characteristics. However, due to the attenuation and variation of AE signals during their propagation in structures, it is difficult to recognize them according to those commonly used AE parameters, such as energy, average frequency, peak frequency, amplitude, and count. Therefore, constructing the deep features of AE signal that do not vary with propagation is of great value for damage identification. As fiber breakage is the most important damage mechanism affecting the load-bearing capacity of CMCs, it's exact identification is much helpful for structural health monitoring of CMC structures. In this paper,the deep features of AE signal generated from A series of experiments were conducted, focusing on the propagation and attenuation of AE signals originating from a singular source of damage. Tensile tests were performed on individual C fibers and SiC fibers to generate AE signals. These signals were collected at various positions along their propagation paths on a C/SIC plate. The collected AE signals were then transformed into 24-dimensional deep features utilizing Mel-cepstral coefficients (MFCCs), enabling the identification of the "timbre" of original AE signal. These deep features remain consistent throughout the entire propagation process. The results are concluded as follows: (1) During the propagation of AE signals from the fracture of C fibers and SiC fibers in CMCs, most of the frequency responses are concentrated in the range of 0-50kHz. (2) The MFCC curves of the AE signals collected at different locations from the same source demonstrate that the extracted deep features exhibit good consistency. (3) The variation trends of the 24-dimensional deep features extracted from the AE signals collected at different positions are similar, demonstrating that the MFCCs can extract the invariant features in the AE signals.

Multi-scale and machine learning-based modeling methods for optimization and design of composites
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MICROMECHANICAL MODELING OF THE VISCOELASTIC–VISCOPLASTIC RESPONSE OF FIBER-REINFORCED COMPOSITES

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ABSTRACT

The demand for fiber-reinforced composites in aircraft components has been steadily increasing due to their improved mechanical properties. However, designing the mechanical properties of composite structures involves time-consuming multiscale computation. As a result, there is ongoing research focused on improving the computational efficiency of multiscale simulations for fiber-reinforced composites. Micromechanical models have shown good predictability with high efficiency when it comes to determining the effective mechanical behaviors based on the mechanical properties of the constituents and the microstructures of the composites. Therefore, these models can be used to replace the simulation of representative volume elements (RVE) in microscopy, leading to improved efficiency in multiscale computation. However, composites with a polymer matrix often exhibit strong nonlinear viscoelastic-viscoplastic responses in the transverse plane. This poses theoretical challenges when it comes to establishing micromechanical models for such composites. This work describes a newly proposed viscoelastic–viscoplastic constitutive model that is used to characterize the effective mechanical behaviors of fiber-reinforced composites based on micromechanical modeling. A homogenization approach is developed in which the effective stress of the fiber-reinforced composite is decomposed into an elastoplastic component and a viscous component. For the elastoplastic component, a bridge model is adopted to characterize the elastoplastic behaviors, while for the viscous component, homogenization theory applied to the time domain is utilized to describe the effective viscous responses. The overall stress for the composite can be obtained by superposing the stress contributions of the two components. The proposed micromechanics-based constitutive model has an explicit form, which contributes to the computational efficiency of the multiscale simulations for the composite structures. Unit cubes with 128 randomly distributed cylindrical fibers of equal size are created as the representative volume element models for numerical validation of the proposed constitutive model. The effects of fiber volume fraction, hardening law, loading condition, and strain rate are considered to comprehensively validate the constitutive model. Experimental results for IM7/8552 carbon fiber–reinforced composite were employed to validate the constitutive model. By comparing the model predictions to the experimental results and numerical observations, the constitutive model was found to provide acceptably good predictions of the viscoelastic–viscoplastic behaviors of the fiber-reinforced composites.

Methods for identification, machine learning, and uncertainty quantification of reduced order models of coupled systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GPT-PINN: GENERATIVE PRE-TRAINED PHYSICS-INFORMED NEURAL NETWORKS TOWARD NON-INTRUSIVE META-LEARNING OF PARAMETRIC PDES

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ABSTRACT

Physics-Informed Neural Network (PINN) has proven itself a powerful tool to obtain the numerical solutions of nonlinear partial differential equations (PDEs) leveraging the expressivity of deep neural networks and the computing power of modern heterogeneous hardware. However, its training is still time-consuming, especially in the multi-query and real-time simulation settings, and its parameterization often overly excessive.

In this talk, we present the recently proposed Generative Pre-Trained PINN (GPT-PINN). It mitigates both challenges in the setting of parametric PDEs. GPT-PINN represents a brand-new meta-learning paradigm for parametric systems. As a network of networks, its outer-/meta-network is hyper-reduced with only one hidden layer having significantly reduced number of neurons. Moreover, its activation function at each hidden neuron is a (full) PINN pre-trained at a judiciously selected system configuration. The meta-network adaptively “learns” the parametric dependence of the system and “grows” this hidden layer one neuron at a time. In the end, by encompassing a very small number of networks trained at this set of adaptively-selected parameter values, the meta-network is capable of generating surrogate solutions for the parametric system across the entire parameter domain accurately and efficiently.

Data science and machine learning applications for composite materials and biomedical engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LETHALITY PREDICTION OF OSTEOGENESIS IMPERFECTA BY A STRUCTURE- AND SEQUENCE-INFORMED GRAPH NEURAL NETWORK

Yen-Lin Chen[*1], Wei-Han Hui[1] and Shu-Wei Chang[1]*

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ABSTRACT

Collagen, one of the most abundant proteins in the human body, plays a huge role in biomechanics, with its health condition greatly influencing biological performances, such as bone strength, skin elasticity, and blood vessel elasticity. Needless to say, any mutation could potentially have profound impact on the subject. Osteogenesis imperfecta (OI) is one of the rare diseases associated with mutation on type I collagen and is characterized by a reduction in bone strength. Its locus of mutation is not a single site, but any of the amino acids along each collagen molecule, which adds to the complexity of the subject. Although recent advances have made possible sequence-based lethality prediction of this disease, its low occurrence rate and large number of possible mutation sites limit the accuracy of these methods. In this work, we merged the structural features of the collagen molecule with its sequential characteristics into a single graph representation of the vicinity of the mutation site, and designed a graph neural network to interpret the lethality point mutations known to induce OI. Our method enhances the accuracy of lethality prediction in the α1 chain and simultaneously extends the prediction to mutations on the α2 chain. A Grad–CAM-based technique is then employed to explain the inferences made by our model. We anticipate the proposed method to pave the way to methods for early on diagnosis and advance our understanding of the pathology at the molecular level.

Microstructures of chemically complex materials and their impacts on material properties from multiscale simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

KINETIC MONTE CARLO SIMULATION OF ATOMIC DIFFUSION BEHAVIORS IN THIN FILM EPITAXY

Yu-an Chen[1], Xin-Yang Zhong[1] and Yu-Chieh Lo[1]*

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ABSTRACT

Kinetic Monte Carlo (KMC) is a kind of simulation method widely used to explore the state transitions on a large time scale. In material science, KMC is a valuable tool for studying the diffusion behaviors of atoms on the surface or inside the materials, such as surface growth and vacancy mobility. In this research, we used KMC method to study the formation of nanowires on vicinal surfaces, aiming to gain insight into the diffusion mechanisms under different conditions and to find the optimal experimental parameters for growing nanowires with large aspect ratios. In addition to showing how to write KMC programs that can be applied to epitaxy simulations, we also tried to improve its shortcomings, turning it into a novel KMC framework called “on-the-fly KMC”. Therefore, the final part of this study demonstrates the introduction of an "on-the-fly" algorithm in the classical framework. The first part involves utilizing the Nudged Elastic Band (NEB) method to calculate energy barriers for different events. To enhance program efficiency, the second part involves using these events to train a machine learning model. Ultimately, machine learning methods are employed to complete the simulation results of epitaxial growth of thin films. The study also discusses some obstacles we may encounter in the future and potential directions for future development.

Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COHESIVE CRACK PROPAGATION MODELING BASED ON THE SELF-STABILIZED VIRTUAL ELEMENT METHOD WITH AN ELEMENT SPLIT STRATEGY

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ABSTRACT

The Virtual Element Method (VEM) [1] does not require geometry mapping, allowing for arbitrary element shapes, not necessarily convex, free of distortion sensitivity. Thanks to these features, especially the flexibility in element shapes and mesh definition, the VEM is particularly suitable for simulating crack propagation in arbitrary directions through the elements. Following the mixed approach proposed in [2], a linear strain model is adopted to obtain an initially self-stabilized model and a more accurate stress field.

In this work, a 2D mixed-mode fracture evolution model is established based on the mixed-VEM coupled with cohesive interface elements, considering two different linear strain models. The crack propagation direction is determined based on the maximum principal stress direction. The linear stress field around the crack tip is smoothed across adjacent elements by a patch recovery technique. The crack is allowed to propagate through a Virtual Element (VE) by adding to the element at least one node and two edges (element-split strategy, see e.g. [3]) separated by a cohesive interface element. The non-convex mixed-VE which is obtained in this way requires a specific stabilization. Both mode-I and mixed-mode numerical examples are simulated, allowing cracks to propagate through the VEs. The crack paths and the force-displacement curves obtained with the proposed model, based on the element-split strategy, show good agreement with the experimental results. These examples and results validate the accuracy and computational efficiency, especially in terms of mesh management, of the present VEM-based fracture evolution model.

Keywords: Virtual Element Method; Linear strain model; Effective cohesive model; Element split strategy; Crack propagation

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PROGRESSIVE FRACTURE PATTERN PREDICTION IN FIBER-REINFORCED COMPOSITES USING GRAPH NEURAL NETWORK

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ABSTRACT

Abstract
Composites have been a material of interest in the aerospace industry because of their superior properties such as high strength-weight ratio and exceptional thermal stability. Understanding the nonlinear process of fracture and damage formation is crucial for enhancing the mechanical performance of these materials. The conventional approach, leveraging finite element methods (FEMs) for damage prediction, encounters limitations. These include the necessity for accurately defined constitutive models and extensive mesh refinement, which often result in computational inefficiencies and potential inaccuracies in complex fracture scenarios. Recent advances in scientific machine learning have opened avenues for more efficient fracture pattern prediction methodologies. For example, a recent data-driven model by Sepasdar et al. [1], employing a deep learning framework with two stacked fully convolutional networks, successfully predicts post-failure stress distribution and failure patterns in composites. However, its static nature limits its application in scenarios where understanding the evolution of fracture patterns prior to ultimate failure is crucial. To bridge this gap, we introduce an innovative approach utilizing MeshGraphNets (MGN), developed by Pfaff et al. [2], for progressive fracture analysis. MGN, operating on a graph neural network architecture designed for mesh-based simulations, employs an Encode-Process-Decode framework. This framework begins with an encoding phase, where the input mesh is transformed into a graph representation. The processing phase then involves iterative message-passing algorithms, updating node and edge embeddings to capture the evolving stress-field dynamics. The decoding phase extrapolates these embeddings to update and predict subsequent mesh configurations, reflecting the progressive fracture patterns. The proposed model is applied to a longitudinal carbon fiber-reinforced polymer (CFRP) composite, selected for its relevance in high-performance aerospace applications. We evaluate the model's efficacy in predicting progressive crack patterns and the full-field von Mises stress distribution over time, offering a significant improvement over traditional methods in computational damage mechanics. The results show the potential to advance the predictive modeling of progressive damage processes in advanced composites.

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Scientific deep learning
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GRAPH OSCILLATORS: PHYSICS-GUIDED GRAPH MODELING OF MASS-SPRING-DAMPER SYSTEMS FOR TRAJECTORY PREDICTION AND DAMAGE LOCALIZATION

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ABSTRACT

Recognizing that a multiple-degree-of-freedom mass-spring-damper system can be viewed as a group of connected nodes, this work presents a novel computational framework that learns such coupled oscillations by a graph, a mathematical structure describing pairwise connections between objects. Further reinforced by an incomplete equation of motion, distributed neural networks and an anti-symmetric coupling constraint, we can learn unknown coupling mechanisms (or nodal interactions in the language of graph models) using limited data. The proposed physics-data-hybrid method demonstrates a promising predictive capability even for unseen control inputs, outperforming three black-box and grey-box counterparts in synthetic and experimental studies. In addition to its predictive capability, the distributed parameterization of nodal interactions allows us to identify local anomalies by evaluating updates after short transfer learning. While limits of the current method exist, it displays the potential of a generalizable and interpretable meta-model for predicting nonlinear trajectories and identifying the system's status.

Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ENGINEERING POROUS COMPOSITES AGAINST IMPACT WITH PARTICLE METHODS

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ABSTRACT

The responses of porous composites to impact loading play an important role in optimizing blast/impact-resistant design scenarios, which have been investigated with different spatial discretization methods at different scales. Molecular dynamics (MD) and the finite element method (FEM) are representative discrete particle and continuous methods, respectively. The Material Point Method (MPM) is a continuum-based particle method that is formulated based on the weak form of the governing equations in a way like the FEM. A challenging task is how to verify and validate multiscale shock responses because impact experiments are limited in spatial nanoscale while nanoscale experiments are limited in high loading rates. Based on the recent research results [Saffarini et al., 2023; Su and Chen, 2023], we are performing a comparative study of shocked porous composite responses with MD and different versions of MPM [Su et al., 2024]. Essential features of the responses at the same spatial scale as obtained with both discretization procedures will be presented in the conference for representative composite systems under impact loading. It appears from the investigation that the MD and MPM solutions are consistent at the same scale. Thus, it become feasible to compare the MD and MPM solutions for verification in multiscale simulation of impact responses. The verified MPM solutions will then be validated against macroscale impact experiments. Future tasks will be discussed to improve the proposed procedure for engineering porous composites against impact loading with particle methods.

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Machine learning for design tasks and inverse problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATION OF AUTOMATIC AND OPTIMAL DESIGN FOR ANTHROPOMORPHIC ROBOTIC HAND BASED ON GENERATING TRAJECTORIES BY ARNN

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ABSTRACT

With the advancement of Large Language Models (LLM) and the emergence of humanoid robots, there is an increasing demand for robots to perform complex tasks involving objects with diverse characteristics. Anthropomorphic robotic hands with a high degree of freedom have become a prominent solution in addressing this challenge. However, achieving both high dexterity and structural simplicity in hand manipulation remains extremely challenging due to current hardware limitations. To address this inverse design issue, this paper proposes a fully automated design method for anthropomorphic robotic hands that can handle uncertain clamped targets. We employ neural networks to predict the possible positions of objects and their feature points within the workspace, enabling us to generate potential finger trajectories for anthropomorphic robotic hands based on these predictions. Finally, we do optimized structure after generating of anthropomorphic robotic hands structure based on the fitting of this predict trajectory. However, the linkage group in the finger of anthropomorphic robotic hands exhibits distinct nonlinear dynamics due to variations in linkage lengths and combination methods. The conventional dynamics process is intricate and challenging to optimize. In this paper, a genetic algorithm is proposed for determining the optimal length of the connecting rod that aligns with the predicted trajectory, enabling identification of individual rod lengths and the best matching mode of linkage groups. Subsequently, these parameters including length and composite mode are incorporated into 3D software to facilitate automated design of an anthropomorphic robotic hand. Finally, using commonly encountered real-life objects as examples, this method is employed for optimization and anthropomorphic robotic hands design after topology those objects; subsequently comparing it with existing release hand schemes validates its effectiveness and superiority.

Advanced computational modelling of wood, wood-based products, bio-composites, and timber structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CONSTITUTIVE MODELLING OF WOOD-BASED MATERIALS

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ABSTRACT

Computer modelling is an essential part in the analysis and design of residential and commercial buildings. It is also a valuable tool in the development and optimisation of wood-based products, connections, and systems. The global interest for use of wood-based products as structural and non-structural components in high-rise and long-span structures is gaining momentum, due to their sustainability and low carbon footprint. A survey shows that practicing engineers are typically unfamiliar with timber structure modelling, and researchers generally lack resources for advanced modelling of timber systems. Recently, a first-of-its-kind modelling guide for timber structures has been developed by more than 100 global experts [1]: web.fpinnovations.ca/modelling, for supporting the application of numerical modelling on analysis and design of timber structures, and development and optimisation of wood-based products and systems.

Wood, unlike steel and concrete, is an anisotropic material. Because of its inherent characteristics, the mechanical behaviour of wood depends on the direction of the grain and the load type. The mechanical properties of wood change as temperature, moisture, and loading time change. Moreover, growth characteristics such as slope of grain and knots significantly affect the mechanical behaviour of wood-based products. Appropriate material models are the fundamental basis of reliable simulations. The constitutive models incorporated in existing general design software packages are often limited, making the software unsuitable for accurately predicting the mechanical behaviour and failure modes of wood-based materials.

In this paper, a comprehensive constitutive model, composed of sub-models for describing the elastic properties, strength criterion, post-peak softening for quasi-brittle failure modes, plastic flow, and hardening rule for yielding failure modes, and densification perpendicular to grain, will be introduced. Modelling considerations on the effects of temperature, moisture content, and loading time will be discussed. Advanced and practical modelling methods and key considerations for wood-based products will be introduced, aiming to support practicing engineers and researchers to become better acquainted with modelling and analysing timber structures.

Recent developments in peridynamics modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THERMALLY-INDUCED FRACTURE IN THE OXIDE SCALE OF T91 FERRITIC/MARTENSITIC STEEL AFTER EXPOSURE TO OXYGEN-SATURATED LIQUID LEAD-BISMUTH EUTECTIC

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ABSTRACT

Ensuring the continuity and stability of the oxide scale to separate T91 steel from lead-bismuth eutectic (LBE) is an effective method for limiting corrosion in the lead-based fast reactor system. In this study, we specifically investigated the impact of cooling thermal stress on the stability and damage of the oxide scales of T91 steel when exposed to oxygen-saturated liquid lead-bismuth eutectic at high temperatures. A corrosion test was conducted on T91 steels exposed to stagnant oxygen-saturated LBE at 500 °C. Experimental results indicated that oxide damage exists without external force, including interface cracks and through-scale cracks perpendicular to the interface. We developed a three-layer peridynamic model of T91-(Fe,Cr)3O4-Fe3O4 to simulate the deformation and failure of oxides under a cooling process from high temperature to room temperature. The simulation results show that a temperature drop of about 200 °C from 500 °C can cause through-oxide cracks in the oxide scale, and subsequent cooling can lead to the propagation of interfacial cracks. Additional modifications were introduced in the model to account for the porosity of the oxide scale. Parametric investigations illustrate the effects of oxide scale thickness and porosity on the resulting crack patterns.

Multiscale modeling of dynamics in complex media and metamaterials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PARAMETRIC ANALYSIS AND DESIGN FOR IMPACT PROTECTION BASED ON FINITE LOCALLY RESONANT METAMATERIAL ARRAYS

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ABSTRACT

Locally resonant mechanical metamaterials (MM) have long attracted research interest due to their rich dynamical behavior and application potential in controlling stress wave propagation. This study analyzes the dynamic response of locally resonant metamaterials under impact loadings and aims to identify optimal MM systems for impact mitigation, with specific considerations on the effect of loadings and boundaries. Traditional studies focus on the properties of periodic systems through idealized periodic setups such as eigenfrequency study and frequency domain scattering analysis. While these intrinsic properties encode important information such as band gaps and wave speeds, they can only predict the scattering response to a certain extent in real world or experimental cases. The effects of domain size, loading, and boundary conditions are as important for understanding the extrinsic behaviors and are vital factors for designing applications with finite metamaterials. To this end, a parametric study is carried out to analyze the energy transfer characteristics, as well as the effects of projectile geometry and material parameters, boundary environment, and the MM design. A multi-fidelity approach incorporating a reduced order model and finite element method is employed to accelerate the computation. The parametric and sensitivity analysis reveals design principles for maximizing MM performance given a loading condition, and also shed lights on developing proper experimental setups that can best highlight and demonstrate the metamaterial behaviors.

Data-driven device and circuits models
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA DRIVEN PAM-4 MODELING WITH GENERATIVE NETWORKS

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ABSTRACT

Data-intensive applications such as artificial intelligence and graph processing require fast data rates to enable edge applications. To that extent, PAM-4 aims to alleviate the present binary or NRZ data transmission issues. As the name suggests, PAM-4 contains 4 distinct logic levels whereas NRZ has 2, enabling it to send double the data of NRZ for the same transmission speed. Using 4 distinct logic levels reduces the noise margin available to recover a symbol; thus, there is a need for accurate simulations during the design process. However, simulations for high-speed receivers work assuming the channel is LTI, leading to overly optimistic results. Further, the receivers contain complex filters to counteract channel impairments to recover the data successfully.

This talk/paper presents a measurement-driven approach for modeling a high-speed PAM-4 receiver. The approach uses conditional generative networks (cGANs), enabling us to create a digital twin of the receiver. The digital twin considers random bitstreams, complex filter settings, and channel conditions containing crosstalk. Though model training is a traditional black box model, we integrate domain knowledge as bathtub curves at different time intervals to improve accuracy.

Once trained, we demonstrate that the model takes under 300 ms to perform inference, which is over 40 times faster than the device connected to a scope. To show the advantage of such a digital twin, pass in a random waveform and use the digital twin as a fast-to-evaluate surrogate to optimize the eye openings. Lastly, we show that the latent space of digital twins based on GANs has physical meaning regarding channel loss and enables the identification of previously unseen cases.

Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADVANCING ONLINE PREDICTIONS IN LASER POWDER BED FUSION: A SCIENTIFIC DEEP LEARNING APPROACH INTEGRATING IN-SITU MONITORING DATA WITH MELT POOL SIMULATIONS

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ABSTRACT

The employment of in-situ monitoring systems in laser powder bed fusion manufacturing has shown potential in tracking and adjusting process parameters. However, existing systems, such as electric sensors and cameras, face significant interference from harsh environmental factors like high temperatures and evaporation plumes, limiting their ability to accurately capture melt pool evolution. While physics-based simulations offer detailed insights into melt pool dynamics, their high computational costs and extensive calibration requirements render them impractical for real-time monitoring and control. This study introduces a scientific deep learning (Sci-DL) model designed to reconstruct 3D melt pool evolution by integrating multi-modal in-situ data with high-fidelity simulations. The model leverages an encoder-decoder architecture, employing convolutional neural networks for image segmentation and feedforward neural networks for universal approximation. To ensure physical accuracy, the model incorporates governing equations of mass and heat transfer, directing the learning process to align with actual physical phenomena. This integration ensures that the prediction is reliable and robust. With extensive offline training, the Sci-DL model allows real-time 3D visualization of the melt pool evolution during the process and potentially enables online control of the manufacturing process. We demonstrate the model's effectiveness in full-field melt pool recovery with several numerical examples, showcasing its ability to efficiently process various combinations of process parameters using limited data.

Numerical modeling of granular and multiphase flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A SIMPLIFIED ROBUST DIFFUSION INTERFACE MODEL FOR ELASTIC SOLID-FLUID INTERACTION

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ABSTRACT

The Eulerian elastic solid-fluid diffusion interface model has been applied to simulate the interaction between elastic solids and fluids. However, there still exists several challenges, for example, the calculation of deformation gradient tensors for each component is computationally expensive, the robustness for dealing with non-conservative volume fraction equation needs to be improved. In this paper, we propose a novel approach that combines a simplified deformation gradient tensors equation with the pressure non-equilibrium six-equation diffusion interface model. First, a common deformation tensor with deviatoric elastic strain equilibrium is suggested to simplify the calculation. Furthermore, a pressure relaxation process is used to achieve pressure equilibrium. The Mie-Gruneisen equation-of-state is adopted as the constitutive equation, and the HLLD Riemann solver is utilized to compute the numerical fluxes. Interfaces are sharpened by the THINC method with the MUSCL reconstruction. The third-order TVD Runge-Kutta method is employed for the hyperbolic time step. The variables are updated by hyperbolic time steps and pressure relaxation steps. The effectiveness and robustness of the model are validated through a series of numerical examples involving solid-fluid interaction, including solid-solid Riemann problems and high-pressure gas-solid interaction.

Key words: diffusion interface model, solid-fluid interaction, pressure non-equilibrium

Recent advances in partitioning method and interface mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INTERFACE LOCALIZATION-BASED EFFICIENCY ENHANCEMENT ON PARAMETRIC VARIATIONS OF LARGE-SCALE DYNAMICAL SYSTEMS WITH MULTIPLE SUBDOMAINS

Seunghee Cheon[*1] and Jaehun Lee*[1]

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ABSTRACT

While the computational approach can leverage efforts to solve various scientific and engineering problems, real industrial engineering applications still require substantial computational resources. For this reason, parametric reduced-order modeling (PROM) approaches have been actively developed for several decades. To achieve efficient computation for these complication systems, the conventional PROM adopts ROM adaptation consisting of the offline and online stages. In the offline stage, the reduced systems are constructed with respect to defined operating points for rapid response of parametric variations performed in the online stage. It is inevitable to consume significant computation for this offline stage data construction. As a solution for the efficient sampling stage, component mode synthesis (CMS) [1] has been suggested for real-world applications involving multiple subcomponents. Based on the concept of domain decomposition, the number of constructed samples is considerably reduced by comparison to full system sampling due to subdomain independence. In addition, the reduced sample systems could be considered in much smaller scale.

Despite the aforementioned benefits of CMS, the interface where is for subdomain synthesis is fully retained without reduction. For sufficient model reduction user aiming, interface reduction [2] is an essential consideration for studies related to CMS. The conventional parametric CMS [3] performs secondary eigenvalue analysis in the online stage. This additional computation, requiring greater computational resources than other basic computations, hinders near real-time operation under multi-query systems. To achieve a highly reduced system without concerning the online stage computation, reduced interface sampling is proposed in this study. Based on the conventional parametric CMS, the solution of the new input parameter is derived by interpolating pre-computed reduced subsystems and interface reduction bases. Additionally, an interface discrimination algorithm is also presented to construct interface samples in semi-localized level. As a result, rapid response for parametric variations is allowed with an affordable amount of offline computation.

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Advanced numerical methods for the modeling and optimization of coupled dynamical systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

OPTIMAL DESIGN OF VEHICLE DYNAMICS USING GRADIENT-BASED, MIXED-FIDELITY MULTIDISCIPLINARY OPTIMIZATION

Hyunmin Cheong[*1], Mehran Ebrahimi[1], Hesam Salehipour[1], Adrian Butscher[1] and Alex Tessier[1]*

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ABSTRACT

In automotive engineering, designing for optimal vehicle dynamics is challenging due to the complexities involved in analyzing the behavior of a multibody system. Typically, a simplified set of dynamics equations for only the key bodies of the vehicle such as the chassis and wheels are formulated based on reduced degrees of freedom [1]. In contrast, one could employ high-fidelity multibody dynamics simulation and include more intricate details such as the individual suspension components while considering full degrees of freedom for all bodies; however, this is more computationally demanding. Also, for gradient-based design optimization, computing adjoints for different objective functions can be more challenging for the latter approach [2], and often not feasible if an existing multibody dynamics solver is used.

We propose a mixed-fidelity multidisciplinary approach, in which a simplified set of equations is used to model the key vehicle dynamics while incorporating a high-fidelity multibody suspension module as an additional coupled discipline. We then employ MAUD (modular analysis and unified derivatives) [3] to combine analytical derivatives based on the dynamics equations and finite differences obtained using an existing multibody solver. Also, we use a direct collocation method for time integration, which solves for both the system trajectory and optimal design variables simultaneously. The benefits of our approach are shown in an experiment conducted to optimize vehicle parameters for both handling and ride comfort. In summary, the current work demonstrates that a gradient-based, mixed-fidelity multidisciplinary design optimization approach provides a scalable solution for tackling a complex vehicle dynamics application.

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MODELING TIME-VARYING PORT-HAMILTONIAN SYSTEMS

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ABSTRACT

As technology advances and engineering challenges become increasingly complex, the need for robust mathematical frameworks to describe and control dynamic systems is more pressing than ever. Port-Hamiltonian modeling, with its emphasis on energy-based formalism [1], provides a powerful paradigm for understanding the inherent structure of physical systems, especially those characterized by nonlinearity and time variability.
Port-Hamiltonian systems are based on the concepts of passivity and nonnegativity in a more structured way. We will explore the relation between those properties and the solution of the Kalman-Yakubovich-Popov (KYP) inequality that is used for the characterization of passivity [2]. In addition, a port-Hamiltonian formulation is presented for time-varying systems.
The main goal of this work is to represent time-varying systems in a structured and psychically meaningful way within the port Hamiltonian framework while achieving good numerical results. In this direction, we present preliminary results on structure-preserving model reduction using Galerkin projection. This results in a more concise representation that can then be used in industrial
applications.
Finally, we show how this formulation is used to model real world applications and how the port-Hamiltonian framework can be used to model nonlinear and time varying systems.

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Advanced materials: Computational analysis of properties and performance
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CONSTITUTIVE MODELING OF THE MULLINS EFFECT IN FILLED RUBBER-LIKE MATERIALS

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ABSTRACT

Filled rubber-like materials are widely used in engineering applications and are known to exhibit a rate-dependent non-linear inelastic behavior and stress-softening, also known as Mullins effect, is frequently encountered. In this work, we characterized and modeled the constitutive response of a handful commercially available filled rubber-like materials. We first perform a set of large-deformation uniaxial experiments at room temperature and at multiple rates. Those experimental findings are used to develop and calibrate a thermodynamically consistent constitutive model, which is then numerically implemented in a finite element package by writing a user material subroutine. The constitutive model is validated by comparing the results of an inhomogeneous experiment and simulation. A key finding of this work is that the mechanisms that cause the Mullins effect appear to be the main drivers of viscoelasticity.

Enabling technologies for digital twins: Model reduction and scientific machine learning
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ACCELERATING PHYSICS SIMULATIONS WITH LIBROM

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ABSTRACT

In decision-making applications, such as parameter study, design optimization, optimal control, and inverse problems, we need to repeatedly solve forward problems. However, subject to the model complexity and the discretization fineness, it may take a long time to complete a single forward simulation with even advanced computing capabilities. Reduced order modeling (ROM) has nowadays become a popular and actively researched computational technique to reduce the computational cost of simulations while minimizing the error introduced in the reduction process. In this talk, we will present recent development of various ROM techniques in the open-source software of libROM, including projection-based nonlinear model reduction, non-intrusive system identification, and indicator-based and interpolation-based local reduced order models. We will demonstrate the capability of libROM to enable accelerated prediction of complex dynamical processes, namely Sedov blast wave, triple-point expansion, Rayleigh-Taylor instability, pore collapse, laser ray tracing, and molecular dynamics.

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Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING PHASE-TRANSFORMATION INDUCED STRAIN LOCALIZATION USING A NEURAL NETWORK ENHANCED REPRODUCING KERNEL PARTICLE METHOD

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ABSTRACT

Reproducing Kernel Particle Method (RKPM) has demonstrated its proficiency in solving problems with extreme strain rates and severe material distortion, especially with the semi-Lagrangian (SL) formulation [1]. However, introducing the discontinuity in the approximation that captures heterogeneity, fracture, or strain localization remains challenging and lacks computational efficiency. Meanwhile, the application of Machine Learning (ML) has gained much attention in computational mechanics, e.g., solving elasticity problems with Physical-Informed Neural Network (PINN). Nevertheless, solving the equation solely by Neural Network (NN) without the aid of the existing numerical method may suffer from low efficiency and convergence issues. Therefore, incorporating NN to enhance the current numerical method, such as RK, has been proposed. A designated NN has been integrated into the RK approximation to enrich the discontinuity locally [2]. On the other hand, specific weights and biases can be derived to represent the analytical forms of the shape function in some well-known numerical methods, such as the Finite Element Method (FEM) [3]. Optimized relocation of the nodal points can also be accomplished to best produce the localized behavior within the minimum computation cost. In this research, a Neural Network (NN) based algorithm that utilizes specifically designed NN blocks to reproduce desired shape functions for the approximation is proposed and developed to better capture the localized behavior in the vicinity of the discontinuity in elasticity problems. Some additional improvements, such as the adaptive nodal refinement, can be made to augment the local behavior of discontinuity further. A set of benchmarks, including fracture process and strain localization due to phase transformation, is utilized to evaluate the proposed method's effectiveness in handling discontinuity in the solution of elasticity.

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Computational mechanics for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

UNVEILING GAS-LIQUID METAL REACTIONS IN METAL ADDITIVE MANUFACTURING USING HIGH-FIDELITY MODELING VALIDATED WITH EXPERIMENTS

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ABSTRACT

Gases in the atmosphere inevitably react with the melt pool during metal additive manufacturing (AM). Oxygen is particularly reactive and excessive uncontrolled oxidation is detrimental, so most machines purge the chamber with inert gases, which can minimize but not eliminate such reactions. Alternatively, some users exploit the gas–liquid metal reactivity as an opportunity to introduce beneficial precipitates into the melt pool (“reactive AM”). However, the gas–liquid metal reaction and mechanisms in both scenarios remain unclear. Experimental works hitherto provide different explanations to the same phenomena. Therefore, this work seeks to clarify the mass transfer process of oxygen during metal AM through high-fidelity modeling by considering the competition between diffusion and chemical reaction, suboxide evaporation, and the influence of the vapor plume. The simulation results, validated with experiments, provide consolidated insights into the oxygen evolution behavior during metal AM. Counterintuitively, higher melt pool temperatures do not necessarily lead to greater oxidation rates during processing. The melt pool has regions of high and low oxygen gains due to temperature-dependent reaction regimes, with concurrent oxygen loss from evaporation of metal suboxides. Thus, the net oxygen flux varies for different materials, and the oxygen content cumulatively changes as multiple tracks are scanned. Overall, this work provides useful guidance to AM community that seek to ameliorate or exploit the inevitable gas–liquid interaction in metal AM. Cost-saving measures may be possible for determining the purity of shielding gas used in AM, and physics-guided measures can be taken to limit or control gas–liquid metal reactions.

Multiscale methods for advanced manufactured materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MICROSTRUCTURAL DEFECTS AND LENGTH-SCALE PROBLEM INVESTIGATION OF AM ALLOYS

Edwin Chiu[*1], John Emery[1], Kyle Johnson[1], Kyle Karlson[1], Thomas Ivanoff[1] and John Mitchell[1]*

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ABSTRACT

The gap between the engineering and microstructural length-scales in additive manufactured (AM) alloys is a challenging obstacle to connecting laboratory analysis with qualification of components. Defects in AM engineering alloys have been observed and well documented and include lack of fusion porosity, gas entrapped porosity, irregular grain shapes and textures, entrapped oxides, grain boundary precipitates, etc. This causes part to part variability in ultimate strength and ductility, making it difficult to qualify built parts. There is a growing literature on the impacts of these microstructural defects explicitly or otherwise in engineering-scale calculations to predict performance. However, bridging the studies of large-scale component and parts with these microstructural studies remain a difficult topic not yet sufficiently explored. With the advancement of AM processing techniques leading to repeatability of certain mechanical and microstructural bulk characteristics, the importance and accessibility of research in this field are of interest and necessity.

In this presentation we study these phenomena using synthetic microstructures generated with the Monte Carlo code SPPARKS [1]that include realistic grain morphology and texture. Our effort focuses on an AM aluminum alloy, and it is informed by data from high fidelity experimental characterization of the material and pursuant performance. This data-driven approach is part of a broader effort to connect the microstructural length-scale to the engineering length-scale for component qualification calculations. We will discuss observations regarding mesh-to-microstructure size ratio, data acquisition methods, and modified boundary conditions necessary to form reliable representative volume element (RVE) models in the presence of strong gradients. We will also report on the comparison of prediction accuracy/reliability of said method and influence of microstructural features known to impact AM component performance.

1. John A Mitchell et al 2023, “Parallel simulation via SPPARKS of on-lattice kinetic and Metropolis Monte Carlo models for materials processing, Modelling” Simul. Mater. Sci. Eng. 31 055001 DOI 10.1088/1361-651X/accc4b

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Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ARTIFICIAL NEURAL NETWORK FOR THE QUALIFICATION OF DIRECT ENERGY DEPOSITION PROCESSES

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ABSTRACT

The objective of this work consists of the development and implementation of an Artificial Neural Network (ANN) for the process optimization of metal Additive Manufacturing (AM) by Direct Energy Deposition (DED).

The in-house software Add2Man developed at CIMNE for the numerical simulation of the AM-DED thermomechanical process is used to analyze the temperature evolution, the melt-pool morphology, and the microstructure features during manufacturing and the following cooling phase. The software is prepared for parallel computing in distributed memory (clusters) and makes use of the most advanced techniques of adaptive meshing (AMR) to ensure the best performance and the highest accuracy.

The novelty proposed in this work consists of taking advantage of Machine Learning (ML) to provide artificial intelligence (AI) to the DED manufacturing process, allowing for the optimization of the process parameters such as the power input, the printing speed, or the dwell time among layers. By adopting for the software the same input as for the DED machines (G-code format), it is possible to faithfully reproduce the power delivery of the laser along its path, as well as the cooling during repositioning pauses, waiting times, etc. The melt-pool volume is used to continuously monitor and modulate the process parameters. In this way, it is intended to add an active and automated control to AM manufacturing, qualifying this technology for its adoption and integration in the industrial manufacturing chain.

Multiphysics and data-driven modeling for cardiovascular biomedicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HYPER-RESOLUTION AND 3D COMPONENT INFERENCE OF FLOW FIELDS IN VENTRICULAR GEOMETRIES USING NEURAL NETWORKS

Marcello Mattei[1], Mackenzie Meni[1], Arianna Issitt[1], Elizabeth Christ[1], Ryan White[1] and Venkat Keshav Chivukula[1]*

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ABSTRACT

Purpose of Study: Intraventricular blood flow is strongly 3-dimensional, but imaging modalities like ultrasound can only capture one direction, is low-resolution and noisy. We created a pipeline that uses neural networks (NN) to (i) apply hyper resolution to a single component of velocity acquired with simulated ultrasound data, and (ii) predict the remaining two orthogonal velocity components in high resolution to obtain the complete 3D hemodynamic patterns
Methods: A virtual dataset of 47 different intraventricular flow profiles for different anatomical left ventricle (LV) geometries implanted with LVAD was generated by via computational fluid dynamics (CFD) simulations in ANSYS Fluent. These 3D high resolution flow profiles were randomly sampled to 5% of their data density to simulate noisy, low-resolution data (such as from ultrasound). The ground truth high resolution data and the low-resolution data were interpolated and padded into 100x100x100 regular grids. A 3D convolutional U-Net NN was developed to map the sparse flow profile of a single component to a full-resolution detailed profile for the same single component. Two secondary NNs of similar architectures were trained to map the hyper-resolution single component profile to the two remaining flow directions in high resolution. 40 flow profiles were used to rigorously train the networks, reserving the rest for testing. Training was performed using a custom loss function incorporating 3D geometrical features from each model and known fluid flow physics. The resulting high-resolution predictions were interpolated back into their original LV space for prediction evaluation and post processing to visualize the hemodynamic patterns.
Results And Conclusions: Our network pipeline successfully reconstructed ventricular flow profiles from low-resolution single components. The hyper-resolution network expanded low resolution components with good agreement between the flow patterns predicted and the ground truth data. Furthermore, the secondary network predicted the other two velocity components successfully. The 3D profile resulting at the end of our pipeline from hyper resolution and component inference was compared with CFD ground truth, showing good agreement in the predicted patterns of the flow, velocity gradients and as well as in its magnitude. Prediction time for each of our NNs was less than 0.25 seconds for a 3D spatial resolution of up to 1 million datapoints per geometry, allowing for near real-time resolution of 3D vectors from a single component in a high-detailed space. Our methodology introduces a novel approach for rapidly expanding three dimensional velocity fields from low-resolution one-dimensional components for hemodynamic evaluation.

Advanced computational mechanics based on data-driven techniques for structure, structural dynamics and aeroelasticity
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADVANCED TIME-SERIES NEURAL NETWORK-BASED ACTIVE NOISE CONTROL APPROACH FOR THE INTERIOR ENVIRONMENT OF MOBILITY

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ABSTRACT

With advancements in eco-friendly electric hydrogen/propulsion and autonomous systems, the field of advanced air mobility, including electric vertical take-off and landing aircraft, drones, vehicles, and other transportation forms, has the potential to transform the aviation industry and future mobility. As technology and research in future mobility progress, there is a growing interest in assessing the environmental impact, particularly the noise from propulsion systems, which significantly affects boarding comfort and human well-being. Therefore, effective noise control is crucial to ensure safety, provide boarding comfort, and integrate these transportation systems sustainably with a quiet interior environment. In this study, we propose a novel approach to the pipeline in the algorithm for active noise control by training a time series neural network for predicting vibroacoustic characteristics using real-world vehicle test data. Then, we investigate the potential application of this approach in active noise control (ANC) techniques aimed at creating an anti-noise signal to cancel out the target noise signal, ensuring a quieter interior environment. The main key of our framework is predicting noise signals using acceleration signal inputs, specifically at the main vibration transmission path in nonlinear road noise environments. Moreover, to address limitations in existing recurrent neural networks, an Inception network is newly introduced, simplifying the architecture to ensure authentic, on-road conditions shape the findings and conclusions. The proposed framework is evaluated using real-world driving test data, reflecting actual conditions such as road surfaces, driving conditions, ambient noise, and vehicle nonlinear structural dynamics characteristics.

Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NONLINEAR NATURAL ELEMENT METHOD FOR FUNCTIONALLY GRADED GRAPHENE-REINFORCED SHELL-LIKE COMPOSITE STRUCTURES

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ABSTRACT

Functionally graded (FG) composite structures reinforced with graphene platelets (GPLs) or carbon nanotubes (CNTs) have been spotlighted as a state-of-the-art structural element in variuous engineering fields due to the excellent properties and the functional designability. For the successful use of these FG nanocomposites, the intensive research activities have focused on the investigation of their mechanical behaviors. However, most studies were focused on the analytical investigation of linear responses of beam- and plate-like structures.

In this context, the current study intends to develope an effecitve and reliable nonlinear numerical method for analyzing the FG graphene-reinforced shell-like nanocomposite structures. But, the curved neutral surface of shell-like structures makes the mathematical derivation more painstaking and the numerical accuracy more difficulty to secure against the numerical locking. Moreover, these nanocomposites are heterogeneous such that both carbon particles and pores are mixed up in the matrix with the specific volume fraction (VF) pattern. And, these VF patterns significanlty affect the neutral surface location and the resulting stiffness matrix.

These nanocomposites are modelled by the VF-based homogenization, and their displacements are expressed by the shear deformation shell theory with the von-Kármán nonlinearity. And, the nonlinear numerical method was developed in the framework of 2-D planar natural element method (NEM), a meshfree method characterized by high-smooth interpolation functions. A geometry transformation between the curved shell surface and 2-D planar NEM grid is introduced to relax the painstaking mathematical job and the troublesome grid distorsion problem. The transverse shear strains are stably interpolated at the tying points to suppress the numerical locking. The nonlinear stiffness matrix is derived by introducing a partial differential operator B_NL and solved by the associated nonlinear iterative schemes.

The developed nonlinear NEM is verified by comparing with other existing solutions, and its dependence on the key factor such as the porosity pattern is examined. As well, the nonlinear behaviors of FG nanocomposite structures such as nonlinear vibration are investigated and discussed.

ACKNOWLEDGEMENTS: This presentation is dedicated to the memory of Professor J. Tinsley Oden to celebrate his lifetime contributions to the computational mechanics. This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (RS-2023-00240618).

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Design beyond optimization: Why, what if, and how much?
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STOCHASTIC DESIGN SENSITIVITY AND OPTIMIZATION OF THERMAL CONDUCTIVITY OF GRAPHENE USING LINEAR RESPONSE THEORY

Song-Hyun Cha[1], Youmie Park[2] and Seonho Cho[*1]*

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ABSTRACT

We obtained the optimal design for the minimal thermal conductivity of graphene by locating isotopes and antidots in the graphene using a gradient-based design optimization method, which requires a stochastic design sensitivity. Due to the divergent characteristics of the design sensitivity analysis in transient dynamics, however, a direct computation of design sensitivity often fails in long time simulations. Thus, the required stochastic design sensitivity is obtained using a linear response theory.

The linear response theory observes the probability variations with small change of Hamiltonian systems near thermodynamic equilibrium. We obtained the stochastic design sensitivity from linear response theory with variation of design parameters. The computed design sensitivity provides reasonable values compared with averaged finite difference results even though long-time simulations. The linear response theory observes the probability variations with small changes of Hamiltonian system near thermodynamic equilibrium.

We obtained the stochastic design sensitivity from the linear response theory with the variation of design parameters. The developed method for stochastic design optimization is employed to reduce the thermal conductivity of graphene. Thermal conductivity is determined via the Green-Kubo expression. The obtained optimal structure is an aperiodic isotope superlattice structure with the antidots located at interfaces. It turns out that the thermal conductivity of the optimal graphene is reduced by 74.5% of the pristine graphene. In general, the acoustic phonons and the low-frequency optical phonons in dispersion curves have a significant impact on the thermal conductivity. Also, the slope of the phonon curves account for the group velocity. We notice that the slopes of the acoustic phonons and the low-frequency optical phonons get decreased as the design optimization progresses. Also, investigating the effects of the stochastic design optimization on the density of states (DOS), the DOS of the optimal model are smaller than that of the pristine one in low-frequency ranges.

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Recent advances in partitioning method and interface mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SUBSTRUCTURING SCHEME FOR EFFICIENT MULTIVARIABLE DYNAMIC REANALYSIS OF DIGITAL TWINS

Geomji Choi[*1] and Seongmin Chang*[1]

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ABSTRACT

Computational analysis, which has emerged with the development of computers, has become an indispensable element throughout various industries. While past computational analyses were primarily used to obtain straightforward results, such as assessing the failure of designed structures under static loads, recent applications have significantly expanded. This expansion includes dynamic analyses, multi-physics analysis, and other interactions analysis. Optimal design problems, as one of their applications, necessitate numerous adjustments to design parameters within specified constraint to achieve the desired result. In another instance, a digital twin utilizes a computer model that closely replicates the appearance and composition of an actual structure to predict its behavior. To obtain precise dynamic responses, the damping ratio also needs to be considered. Iterative computations are essential for implementing such precise computer models. Consequently, the demand for iterative analysis is increasing in many fields, which results in a significant increase in the computational resources and time costs required for analysis. Hence, the development of analysis techniques is needed to derive results efficiently.

In this study, we propose a dynamic reanalysis technique to efficiently perform iterative analyses. In the proposed approach, the entire analysis model is divided into multiple substructures based on degrees of freedom. This substructuring scheme enables a reduction in the size of the analysis model, facilitating rapid and efficient analysis. Additionally, the analysis process was divided into offline and online stages. During the offline stage, formulas that remain constant throughout the analysis and are unrelated to design variables are calculated in advance. Since the majority of the resource intensive computations occur during the offline stage, this stage accounts for most of the analysis time. In the online stage, formulas that vary based on design variables are computed. At this stage, computations proceed rapidly. This separation of the analysis process leads to efficient performance in reanalysis, as it requires calculations only from the online stage. The efficiency and accuracy of the proposed method were verified through numerical examples. Furthermore, the ongoing research is extending the applicability of the proposed method to dynamic problems involving damping ratios.

Modeling and simulation of advanced manufacturing processes for metals
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ARTIFICIAL INTELLIGENCE FOR RESIDUAL STRESS PREDICTION AND MACHINING PATH OPTIMIZATION WITH THE EXTRUDED ALUMINIUM ALLOY

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ABSTRACT

The residual stress in manufacturing of material itself and post-processing to manufacture the aerostructure component has been a crucial issue for the dimensional accuracy of the manufactured aerostructure component. In this research, the application of artificial intelligence has been introduced for the prediction of residual stress and machining path optimization for the 2xxx series aluminium alloy which is used for aerostructure components. The Bulk Residual Stress (BRS) which is induced by quenching after extrusion was predicted by the ANN model with respect to geometry of material and quenching parameters. The Machining-Induced Residual Stress (MIRS) was predicted by the simple regression model with respect to machining parameters. The data set for each residual stress prediction was prepared by using finite element simulation and experimental results where contour and X-Ray Diffraction (XRD) methods were used for the experiment of the residual stress. Both BRS and MIRS were applied into finite element simulation for the distortion prediction of machining without any fracture model to describe element deletion in machining. In the simulation, the BRS was initially mapped into the extruded material with its geometry and quenching condition. Based on the machining parameters such as tool, feed rate, width of cut, and RPM, the MIRS come to be inserted into the integration points of the element which is located machined surface. Then, through the additional simulation time step to satisfy the force equilibrium which is violated by the BRS and MIRS, the machining-induced distortion could be predicted only by the BRS and MIRS whereby it is possible to perform numerically efficient finite element simulation for the prediction of machining-induced distortion. As far as machining path optimization is concerned, since MIRS includes the machining process parameters, XGBoost regression model was adopted because of its feature which combines several decision tree models to give the best prediction and shows excellent prediction for small datasets.

Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DIFFERENTIABLE THERMOMECHANICAL SIMULATION FOR RESIDUAL STRESS OPTIMIZATION IN ADDITIVE MANUFACTURING

Jin Young Choi[*1], Shuheng Liao[2], Tianju Xue[3] and Jian Cao[1]*

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[2]*Massachusetts Institute of Technology*
[3]*Hong Kong University of Science and Technology*

ABSTRACT

The rapid heating and cooling cycles in metal additive manufacturing (AM) processes induce residual stress that can lead to build failure and dimensional inaccuracies. The experimental measurement of residual stress can be costly and time-consuming. To address this, we present a differentiable thermomechanical simulation for automatic optimization of residual stress by adjusting the input laser power. The code is written on top of Google JAX for its high-performance computing with automatic differentiation capabilities. We employ a finite element method (FEM) to solve the thermal field, combined with an elastroplastic solver for residual stress computation. Examples are demonstrated for the directed energy deposition (DED) AM process, showing reduced residual stress in the final part with the optimized laser input. This work enables the inverse design of process parameters to eliminate distortion and residual-stress induced fracture in AM. Our code is made available to the community to facilitate collaborative research.

ON-THE-FLY DYNAMIC MODE DECOMPOSITION

Seung Won Suh[1], SeungWhan Chung[2], Peer-Timo Bremer[2] and Youngsoo Choi[2]*

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ABSTRACT

The on-the-fly reduced order model concept becomes particularly appealing when dealing with a high-dimensional parameter space. In the realm of time-dependent simulations, this approach initiates with a full order model and concurrently trains a reduced order model as solutions from the full order model are collected on the fly, serving as dynamic training data. Subsequently, the trained reduced order model can replace the full order model if it proves trustworthy, significantly accelerating the simulation process. To assess the trustworthiness of the reduced order model, an indicator is crucial. One evident indicator involves utilizing the residual norm, computed by applying the reduced order model's prediction field to the corresponding governing equations. A high residual norm signals a potential lack of trustworthiness in the trained reduced order model, while conversely, a low residual norm suggests reliability.

While there have been successful implementations of on-the-fly projection-based reduced order models in design optimization [1,2], relatively few have been directly applied to time- dependent problems. Moreover, there appears to be a scarcity of on-the-fly dynamic mode decomposition (DMD) approaches, if any at all. Extending the on-the-fly reduced order model to the DMD framework holds great promise, given that DMD requires less interaction with the physics solver compared to projection-based reduced order models. Additionally, its compatibility with time-dependent problems makes it a natural choice.

Our contribution to this field involves the development of an on-the-fly DMD approach [3]. Leveraging the efficiency of incremental singular value decomposition, our method has demonstrated a notable speed-up of 4.4x compared to the corresponding low-fidelity full order model. This acceleration is achieved while maintaining a solution accuracy similar to that of the full order model, specifically in the context of Navier–Stokes flow around cylinder simulations.

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Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MAPPED MPM FOR SOIL-STRUCTURE INTERACTIONS: CAPTURING SHARP GRADIENTS WITH UNIFORM BACKGROUND GRIDS

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[1]*KAIST*

ABSTRACT

The material point method (MPM) has become a popular means for computational simulation of highly deforming soils interacting with various “structures” such as foundations, penetrometers, and machines. A common and significant challenge in these MPM simulations is how to address sharp gradients in the displacement fields around the soil-structure interfaces with computational efficiency. The existing MPM simulations handled such sharp gradients through the use of locally refined background grids. Unlike meshes in the finite element method, however, local refinement of background grids in MPM are very complicated and restricted to certain types of basis functions or updated schemes. Here, we present a new MPM formulation--the mapped MPM--that can efficiently capture sharp gradients with a uniform background grid. The central idea is to use the method of auxiliary mapping–-a technique that reparameterizes the given problem in a parametric domain where sharp gradients become much smoother. The performance of the mapped MPM is demonstrated through various numerical examples with a focus on soil-structure interaction problems.

Data science and machine learning applications for composite materials and biomedical engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN INVESTIGATION OF THE MECHANICAL BEHAVIOR OF RE-ENTRANT AUXETIC STRUCTURES

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ABSTRACT

Auxetic structures exhibit exceptional mechanical properties stemming from their negative Poisson's ratio. This provides advantages in fracture resistance, energy absorption, and indentation resistance. Among various auxetic structures, re-entrant structures have attracted much research attention due to their tunable behavior and lightweight structural properties. This makes them promising candidates for wide applications across fields such as civil engineering, military equipment, biomedical design, and sports protection. In exploring the performance of re-entrant designs, previous studies have focused on geometrical variables and stiffness gradients by varying wall thickness or altering aspect ratio throughout the structure's height. In this study, we start with classical re-entrant structures and use Finite Element Method to investigate the effect of geometrical parameters, including thickness, aspect ratio, zig-zag angle, repeat unit, and the stiffness gradient of materials under mechanical testing. Stress-strain curves and specific energy absorption are evaluated, as well as investigating deformation processes. We also examine the material response during the compression test with higher compression speeds and compare the dynamic deformation against the static one. Additive manufacturing and experiments are also conducted to compare simulation findings. Our results reports how geometrical variables and gradient design effects the mechanical properties of re-entrant structures. This demonstrates that for wide applications of auxetic structures, response under specific loading conditions must be thoroughly investigated. Our study provides a comprehensive simulation procedure to expand the analysis of structure deformation from low-speed to high-speed and dropping tests, validated through comparison with experiments. With the inherent mechanical benefits of auxetic structures and the insights from our study, we can potentially expand applications into broader protective equipment domains.

Data-driven approaches for solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE DEVELOPMENT OF A CONSTITUTIVE NEURAL NETWORK APPROACH FOR MULTISCALE FRACTURE-TO-DAMAGE MODELLING

Yu-Chun Chou[1], Wen-Yi Hsieh[1], Yu-Zhen Li[1], Tsung-Yeh Hsieh[1], Tsung-Hui Huang[1] and Po-Yu Chen[1]*

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ABSTRACT

A multiscale fracture-to-damage model has been developed to establish a connection between micro-scale fracture mechanics and macro-scale damage evolution [1]. While this model effectively assesses material failure across various scales, it requires intricate problem-solving for microcracks, leading to computationally intensive efforts, like direct numerical simulation (DNS), confined by specific microstructures, e.g. microscopic defects, heterogeneities, and micro-pores. The dimension of the problem often compounds the computational cost due to the curse of dimensionality. Recent offline-type homogenization approaches [2], employing neural network training with a pre-trained model on representative volume elements (RVEs) of the microstructure, have proven effective on online macro-scale simulation. However, conventional artificial neural networks (ANN) may lack accuracy during the extrapolation of data from the offline training dataset. To overcome these challenges, our study introduces an enhanced constitutive artificial neural network (CANN) structure [3] for multiscale fracture-to-damage modelling. The proposed methodology can efficiently compute macro-scale damage evolution from micro-scale fracture or crack accumulation via a derived energy bridging equation, effectively mitigating extrapolation issues in online simulations. The resulting homogenized surrogate model is applicable in macroscopic scenarios with coarser mesh resolutions, significantly enhancing computational efficiency. Validation of this approach involves solving benchmark problems and comparing results not only with DNS but also with the conventional NN method, showcasing superior computational efficiency and efficacy. The proposed enhanced constitutive neural network framework offers a robust solution for overcoming challenges in multiscale modelling of damage in engineering materials.

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Multi-physics and multi-scale simulations with the coupling library preCICE
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A QUICK INTRODUCTION TO THE COUPLING LIBRARY PRECICE AND THE MINISYMPOSIUM

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ABSTRACT

This talk will open the minisymposium and introduce the main concepts of the open-source preCICE coupling library for partitioned, black-box, multi-physics and multiscale simulations. For a longer introduction, join the short course W24-08 on preCICE on July 21.

preCICE enables the efficient, robust, and parallel coupling of separate single-physics solvers. This includes, but is not restricted to fluid-structure interaction. preCICE treats these solvers as black-boxes and, thus, only minimally-invasive changes are necessary to prepare a solver for coupling. Ready-to-use adapters for well known open-source solvers, including OpenFOAM, SU2, CalculiX, FEniCS, and deal.II, are available, while the core library is included in the xSDK ecosystem. The software offers methods for equation coupling, fully parallel communication, data mapping, and time interpolation schemes. The minisymposium brings together users and developers of the software. It enables the exchange of users among themselves, which otherwise would not know much of each other. Furthermore, the developer team can get direct feedback from users, who they sometimes only know from forum conversations. Lastly, the software and its capabilities can be presented to others in a full and broad sense as not only the developers talk about their software, but also users report on experiences. Recent work focuses on extending preCICE towards multi-scale coupling, higher-order mapping, and applications other than fluid-structure interaction. For more information, please visit https://precice.org/.

Multiscale computational and data-driven approach of advanced materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COARSE-GRAINED MOLECULAR DYNAMICS MODEL FOR MULTICOMPONENT ALLOY SYSTEMS USING NEURAL NETWORKS

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ABSTRACT

Cold-sprayed deposition of high-entropy alloys (HEAs) offers an exciting avenue for developing new metal coatings with high wear and corrosion resistance. In the cold-spray process, micron-sized HEA particles are deposited on a substrate at high velocities, leading to large plastic deformation and particle-substrate bonding. The ability to tune the composition of the HEA being deposited has the potential to develop optimized and use-case specific coatings. However, the large compositional design space makes optimizing properties an onerous experimental task. Hence, accurate and fast simulations of HEA cold-spray deposition would be highly valuable. Simulating this process poses two major challenges: 1) The molecular composition must be an input to the model to allow for optimization, and 2) the model must reach micrometer and larger scales to capture the deposition process. To address these challenges, we developed a coarse-grained molecular dynamics method (CGMD). Although several CGMD models for single-element alloys have been developed, building coarse-grained models of multicomponent systems like HEAs remains a significant challenge. For multicomponent systems, the structural coarse-graining based on neighboring atoms leads to an exponentially-large number of coarse-grained particle types. To address this issue, we train a neural network to assign a finite set of coarse-grained particle types based on the elemental composition of the local environment. Then, the coarse-grained interaction potential of each particle type is given by training a Behler-Parrinello-like neural network (BPNN) on all-atom simulations. The coarse-grained model thus retains the compositional information of the underlying all-atomic model while allowing larger length and timescales to be reached. This will facilitate further studies of the microstructural mechanisms driving the deformation of cold-spray particles impacting a substrate.

Computational models and methods for predicting cancer progression and treatment response
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTATIONAL MODELING GUIDED PREDICTIVE ADAPTIVE RADIOTHERAPY (PART) FOR HIGH GRADE GLIOMA

David Hormuth II[1,2], Maguy Farhat[3], Holly Langshaw[3], Mihir D. Shanker[3,4], Wasif Talpur[3], Sara Thrower[3], Jodi Goldman[3], Thomas Yankeelov[5] and Caroline Chung[3]*

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[2]Livestrong Cancer Institutes
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ABSTRACT

Radiotherapy (RT) for high-grade gliomas is currently planned using anatomical MRI data collected either shortly after the maximal safe resection or as a dedicated MR simulation to plan the radiation treatment. This approach fails to capture the biological heterogeneity when defining the target volumes at this baseline timepoint and does not even attempt to measure the spatial-temporal heterogeneity in response to RT until the multi-week treatment course is completed. There have been mounting evidence that target delineation can be improved with multiparametric MRI (mpMRI) and even multimodal imaging; however, taking these just at baseline would not address any spatio-temporal responses to RT. By leveraging biology-based mathematical models, it is possible to personalize the predictions for each patient to describe the intratumoral dynamics of response [1]. In this study, we leverage data from patients enrolled in a prospective study evaluating the changes of the tumor using weekly multi-parametric MRI (mpMRI) that provide anatomical diffusion and perfusion information. We utilize the data collected up to week 3 of RT to personalize a biology-based mathematical model of response for each individual patient to then predict response and progression at the end of therapy. This patient-specific approach was able to achieve accurate predictions of response at both the tumor and voxel levels by the end of radiotherapy and even at 1 month following radiotherapy. By integrating mpMRI data with biology-based mathematical models, we can introduce the concept of predictive adaptive radiotherapy (PART) based on the anticipated change in regional tumor activity in order to better delineate the biologically active regions of tumor and improve outcomes.

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Advanced machine learning methods for multiscale modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NONPARAMETRIC MATERIAL MODEL-BASED FEA WITH GPU FOR FASTER AND ACCURATE NUMERICAL ANALYSIS

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ABSTRACT

Finite Element Analysis (FEA) has been extensively implemented in numerical analysis methodology for a long time. However, defining the idealized model for newly developed material with a complex stress-strain relationship based on experiments was challenging, many researchers suggested implementing a machine learning algorithm to resolve the issue. Various algorithms can be adopted to define the representative uniaxial stress-strain material model from the test data, but applying the same method to another material, mostly concrete and steel, requires extensive parameter tuning or algorithm modification. As a result, creating a nonparametric model which can be easily applied to various materials should be investigated. This research defines the Gaussian Process Regressor (GPR) model based on the Radial Basis Function (RBF) kernel directly from the experimental dataset on steel and concrete materials. However, with the GPR-based material model, computational load increases drastically especially using the implicit solver approach. To resolve the computational pressure of the numerical procedure, parallel processing should be considered, and hardware acceleration with the Graphics Processing Unit (GPU) should be performed for even further speedup. The GPU acceleration of the implicit FEA was introduced into the in-house code largely based on the layered approach originally suggested by Owen and Hinton(1980). GPUs can act as hardware accelerators with massively parallel processing units and strength over linear algebraic operations with a CUDA interface.

A nonlinear implicit FEA of two Reinforced Concrete (RC) beams under flexural bending was performed on the accelerated FEA to mitigate the high computational load that comes from both the GPR material model and implicit layered FEA procedure, and results were compared to the experimental result and numerical analysis result using the conventional constitutive material models. The load-displacement response of the beams corresponded with the experimental data, especially the load at the yielding point of the rebar showed less than a 2.28% difference, and the ultimate load showed less than a 1.55% difference. The GPR-based material model showed less sensitivity over the load step configuration and typical sensitivity over the mesh size. The suggested procedure exclusively performed a linear algebraic operation on the GPU, scaling up to 210,000 DOFs with 24GB of GPU memory space. The speedup of acceleration with benchmark was up to 6 times in terms of wall clock time and showed a linear trend of time consumption increase along with the increase of DOFs, while the non-accelerated or non-optimized program showed a polynomial increase.

Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INFLUENCE OF AGGREGATE TYPES ON MECHANICAL, THERMAL, AND DURABILITY PROPERTIES OF LIGHTWEIGHT AGGREGATE CONCRETE

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ABSTRACT

Lightweight aggregate concrete (LWAC) is a material widely employed in the building and construction industry due to its advantageous characteristics, including low density and excellent insulation properties. LWAC exhibits significantly higher porosity compared to conventional concrete due to the incorporation of porous lightweight aggregates. The choice of lightweight aggregates profoundly impacts the physical properties of LWAC, emphasizing the necessity of studying their influence on material strength and durability. To address this, the study introduces concrete mix designs within two distinct theoretical density categories. Each category maintains a consistent composition, with the only variable being the type of lightweight aggregates utilized: expanded glass, expanded clay, and foam glass. These expanded lightweight aggregates are lightweight and exhibit lower thermal conductivity and water absorption than normal aggregates. The study assesses the thermal conductivity and compressive strength of lightweight concrete specimens through experimental and numerical evaluations. Additionally, the pore characteristics and durability-related properties, including sorptivity, open water porosity, and water penetration depth, were investigated. To gain deeper insights, a permeable index, tortuosity, is examined through a numerical method employing X-ray micro-computed tomography (micro-CT). The findings conclusively demonstrate that the choice of aggregate types significantly impacts the strength, thermal conductivity, and durability attributes of LWAC and strongly correlates with their pore structures. Among the assessed aggregate types, expanded glass emerges as the most favorable material in terms of mechanical and permeability characteristics. This systematic approach employed in the study provides a valuable framework for assessing LWAC properties. Although controlling the pore structures of aggregates remains a challenge, the tools utilized in this study to investigate material characteristics can effectively be employed for further examination and development of lightweight concretes with advanced material performance.

TRAIN SMALL, MODEL BIG: SCALABLE ROBUST PHYSICS SIMULATOR VIA REDUCED ORDER MODELING AND DOMAIN DECOMPOSITION

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ABSTRACT

Numerous cutting-edge scientific technologies originate at the laboratory scale, but transitioning them to practical industry applications can be a formidable challenge. Traditional pilot projects at intermediate scales are costly and time-consuming. Alternatives such as E-pilots can rely on high-fidelity numerical simulations, but even these simulations can be computationally prohibitive at larger scales. To overcome these limitations, we propose a scalable, component reduced order model (CROM) method. We employ Discontinuous Galerkin Domain Decomposition (DG-DD) to decompose the physics governing equation for a large-scale system into repeated small-scale unit components. Critical physics modes are identified via proper orthogonal decomposition (POD) from small-scale unit component samples. The computationally expensive, high-fidelity discretization of the physics governing equation is then projected onto these modes to create a reduced order model (ROM) that retains essential physics details. The combination of DG-DD and POD enables ROMs to be used as building blocks comprised of unit components and interfaces, which can then be used to construct a global large-scale ROM without data at such large scales. This method is demonstrated on the Poisson and Stokes flow equations, showing that it can solve equations about 15−40 times faster with only $\sim$ 1% relative error, even at scales 1000 times larger than the unit components. In this work, CROM is further extended toward nonlinear physics such as Navier-Stokes equation, where it is demonstrated to be amenable to hyper-reduction methods such as empirical quadrature points.

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A PHYSICALLY BASED REDUCED ORDER METAMODEL FOR PARAMETRIC COMPUTATIONAL STUDIES OF LOCAL POST WELD HEAT TREATMENT

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ABSTRACT

Post-welding heat treatment (PWHT) is a crucial procedure in nuclear industries, particularly for large welded components, intended to relax residual stresses and stabilize microstructural effects. Precise control of PWHT parameters is essential to achieve the most relaxed stress zones while minimizing the impact on other parts of the components. Finite element (FE) simulations provide a valuable framework for comprehending the influence of underlying parameters on the mechanical response of components during PWHT. However, the application of Direct Numerical Simulations (DNS) is constrained in this context due to the non-linear nature of elasto-visco-plastic material behavior and the high dimensionality associated with parametric studies in PWHT.
This study proposes a novel approach by integrating FE simulations with a posteriori Reduced Order Model (ROM) to construct a metamodel capable of real-time reproduction of the 4D space-time mechanical fields during the PWHT process, eliminating the need for DNS reruns. The ROM is founded on a sparse High Order Proper Generalized Decomposition (HOPGD) (Lu Y., June 2018). Notably, the ROM modes are constructed with constraints derived from thermodynamic equations and the evolution equations from material modelling. Another distinguishing feature is the sampling strategy, which can be implemented as a random sparse (Ibáñez Pinillo, 2018).

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DEVELOPMENT OF A DESIGN METHODOLOGY FOR SLENDER CARBON-REINFORCED CONCRETE COLUMNS IN AXIAL COMPRESSION BASED ON EC3

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ABSTRACT

Continuous advancements in the field of concrete construction have led to innovative technologies, including carbon-reinforced concretes and ultra high-performance concretes. The engineering utilization of these innovations will in future lead to the construction of slender components and structures with high load-bearing capacities and stiffnesses compared to conventional reinforced concrete structures. The resulting lightweight design not only contributes to resource efficiency but also has positive effects on reducing CO2 emissions by reducing the amount of construction materials needed.
Despite the clear advantages of such innovative material composites, challenging load-bearing and deformation behavior emerges in slender carbon-reinforced concrete components, indicating potential stability issues. To address this concern, current research is dedicated to experimental and analytical investigations of the structural behavior and failure of slender components in compression made of carbon-reinforced concrete, aiming to enhance our understanding of stability-related aspects.
Stability phenomena, such as the buckling of columns, are extensively researched and well-known in steel construction. In Eurocode 3, there is a concept integrated for the calculation of the buckling resistance of steel members, which is based on an empirical-analytical approach. This concept is built on numerous experimental studies on various columns, from which the European buckling curves were derived.
This article focuses on a specific approach to derive a practical design procedure for carbon-reinforced concrete columns in compression based on results from the literature. The proposed methodology follows the proven design concept of steel construction, where the (plastic) resistance of the cross-section for uniform compression is reduced by a reduction factor χ. The advantage of this design principle is that the verification of the cross-sectional capacity is expanded by only one factor to consider buckling appropriately. To enable such an approach for slender carbon-reinforced concrete columns, buckling curves are derived, related slenderness limits and adjustment factors are determined. It is suggested to relate the capacity of the column to a slenderness-related strength at $\lambda_{lim} = 25$ instead of the uniaxial concrete compressive strength ($\lambda << 25$). In this way, a general representation of buckling curves is achieved, which can be applied to a broader range of columns. The overarching goal is to contribute to the development of safe and efficient construction methods with carbon-reinforced concrete, promoting the application of these innovative material composites and facilitating their integration into construction practices.

NONLINEAR SPARSE BAYESIAN LEARNING OF SEMI-EMPIRICAL MODELS IN AEROELASTICITY AND INFECTIOUS DISEASE MODELLING

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ABSTRACT

The use of the nonlinear sparse Bayesian learning (NSBL) algorithm [1] to alleviate overfitting in physics-based models is considered for two diverse applications. The NSBL methodology presents a nonlinear extension to sparse Bayesian learning/relevance vector machines, which results in a semi-analytical framework for automatic discovery of the data-optimal nested model. NSBL permits the modeller to assign priors to parameters that are known to be relevant a priori, while inducing sparsity among potentially irrelevant parameters through the use of automatic relevance determination priors.

In the first application, we study the use of NSBL in nonlinear aeroelasticity. For a two degree-of-freedom pitch-plunge airfoil undergoing limit cycle oscillations (LCO), a semi-empirical aerodynamic model consisting of a polynomial expansion of its displacements and velocities is proposed. This model is grounded in physics as some of the terms may be interpreted as stiffness-type and damping-type terms. However, not all terms carry such interpretations; they may contribute to the data-fit of the model but conversely, they may also contribute to overfitting. NSBL is leveraged to alleviate overfitting, particularly in the data-driven component of the model. This was previously demonstrated for a single degree-of-freedom
pitching airfoil, showcasing NSBL's ability to recover the optimal model nested inside an over-parameterized model by comparison with the standard Bayesian model selection [2].

In the second application, NSBL is deployed for the calibration of compartmental models in infectious disease modelling. Although compartmental models have a mechanistic interpretation, deterministic models with time-invariant parameters innately lack the ability to capture the disease dynamics observed over the multiple waves of the COVID-19 pandemic. With lockdown measures and restrictions on movement affecting disease transmission, calibrating compartmental models using both public health data and mobility data collected from cell phones [3] within the NSBL framework can lead to improved predictions of disease spread.

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APPROXIMATION OF ACOUSTIC BLACK HOLES WITH A STRESS-VELOCITY FORMULATION AND CORRECTED WITH ARTIFICIAL NEURAL NETWORKS

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ABSTRACT

Wave propagation in elastodynamic problems in solids often requires fine computational meshes. In this work we propose to combine stabilized finite element methods (FEM) with an artificial neural network (ANN) correction term to solve such problems on coarse meshes. Irreducible and mixed velocity-stress formulations for the linear elasticity problem in the frequency domain are first presented and discretized using a variational multiscale FEM. A non-linear ANN correction term is then designed to be added to the FEM algebraic matrix system and produce accurate solutions when solving elastodynamics on coarse meshes. As a case study we consider acoustic black holes (ABHs) on beams and plates. ABHs are traps for flexural waves based on reducing the structural thickness according to a power-law profile at the end of a beam, or within a two-dimensional circular indentation in a plate. For the ABH to function properly, the thickness at the termination/center must be very small, which demands very fine computational meshes. The proposed strategy combining the stabilized FEM with the ANN correction allows us to accurately simulate the response of ABHs on coarse meshes for values of the ABH order and residual thickness outside the training test, as well as for different excitation frequencies.

Numerical modelling of composite materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INVESTIGATING COLD COMPACTION OF AL-TIB2 AND AL-SIC POWDER MIXTURES USING FINITE ELEMENT MODELING VALIDATED BY COMPACTION EXPERIMENTS

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ABSTRACT

In recent decades, composite materials based on a metallic matrix reinforced with ceramic particles have replaced traditional monolithic alloys in many applications in the aerospace, automobile, and nuclear industries. These composites offer the potential of enhanced thermal and mechanical properties and greater durability in service. An attractive method for fabrication of metal-ceramic composites is the use of cold compaction of a metal-ceramic powder mixture followed by sintering at high temperatures. During the compaction stage, the time dependent hydrostatic stress at each material point, governs the final density distribution of the component. Large density gradients can result in defective components with low thermal conductivity and reduced ductility and strength. As a consequence, predicting the density distribution during the compaction stage is critical. Although many analytical models can provide average values of the compact density, due to the complex non-linear nature of the compaction process, numerical methods must be utilized to obtain local values of density.

This research focused on investigating the cold compaction process of Al-TiB2 and Al-SiC powder mixtures (0-15% volume fraction of TiB2 and SiC in the Al were considered) using finite element analysis in conjunction with compaction experiments. The powder mixture was assumed to behave like a porous media and was modeled using the Gurson-Tvergaard-Needleman (GTN) approach. A density dependent elastic response of the powder mixture was also incorporated using a user defined sub-routine in the commercial code ABAQUS. Convergence studies were used for solution verification and compaction experiments were used to both identify the GTN model parameters and to validate to computational models. By comparing the computations to the compaction experiments, it is demonstrated that a density dependent elastic response is required in order for the GTN model to accurately represent the observed initial part of the compaction curve where the relative density is low. The study also reveals that the GTN model parameters q1 and q2 can be correlated to the volume fraction of the ceramic reinforcement particles. From a practical point of view it is also shown that increasing the volume fraction of the ceramic reinforcement, although increasing initial powder density results in greater local density gradients.

Modeling and simulation of advanced manufacturing processes for metals
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATION OF A TRANSIENT HEAT SOURCE MODEL TO PART-SCALE SIMULATIONS OF AM

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ABSTRACT

In the field of additive manufacturing (AM), continuum melt pool models play a crucial role in understanding the process-structure-property relationships in AM parts. These models scale simulations to relevant lengths and time scales by employing volumetric source terms to approximate the heat input from a moving laser and its impact on melt pool dimensions. Here, we address inherent limitations of conventional continuum melt pool models, which predominantly rely on static heat source geometries calibrated against single-track experiments. This conventional approach often leads to inaccuracies in predicting dynamic melt pool shapes influenced by varying scan strategies and part geometries, resulting in notable discrepancies in the prediction of local defects (such as lack-of-fusion and keyhole porosity) and microstructural features compared to empirical data.

To overcome these challenges, we introduce a refined two-parameter heat source model that independently controls the distribution of absorbed power and the shape of the heat source, better approximating the effect of vapor cavities on melt pool shape. This parameterization significantly improves the prediction of melt pool geometries across a wide range of transient thermal conditions with negligible additional computational expense compared to existing models. Importantly, the proposed model leverages empirical evidence from previous experimental studies that establish causal links between melt pool dimensions and laser absorptivity in laser powder bed fusion (LPBF), reducing the reliance on abstract mathematical parameters and thus improving the model’s adherence to physical phenomena. The calibration of both model parameters is demonstrated to be straightforward using an automated surrogate-based approach based on Bayesian statistics.
Implemented within the OpenFOAM finite volume framework, the model's adaptive mesh refinement (AMR) and CPU load-balancing facilitate the investigation of melt pool conditions at the LPBF part scale. Its application within the Manufacturing Demonstration Facility (MDF) at Oak Ridge National Laboratory (ORNL) enables the use of in-situ build data collected from actual AM machines to automate the deployment of simulations and the collection of their predictions in a digital twin framework. This streamlined approach is believed to narrow the gap between experimental observations and theoretical predictions of process-structure-property relationships at the part scale.

Computational models and methods for predicting cancer progression and treatment response
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PATIENT-SPECIFIC BREAST TUMOUR MODEL FOR PREDICTING RESPONSE TO NEOADJUVANT CHEMOTHERAPY

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ABSTRACT

Neoadjuvant chemotherapy (NACT) is a common treatment option for patients with locally advanced breast cancer. However, only 39% of these patients achieve pathological complete response and up to 12% experience no response at all. Non-responsive patients suffer the side-effects of NACT without reaping the benefits. It is essential to identify non-responsive tumours as early as possible to enable clinicians to discontinue the unsuccessful NACT and proceed with alternative treatment.

To this aim, we propose a light and efficient mathematical model of tumour spatiotemporal evolution in response to NACT, personalised with data from magnetic resonance imaging (MRI). This evolution is described by reaction-diffusion equations parameterised by the spatially varying tumour volume fraction. We have implemented this model in FEniCSx, an open-source platform for solving partial differential equations.

We use diffusion-weighted (DW-) and dynamic contrast-enhanced (DCE-) MRI acquired from patients before, during and after NACT to personalise the model. The DCE data are used to identify the tumour and derive spatially varying maps of the extended Kety-Tofts model parameters volume transfer constant Ktrans, extracellular extravascular volume fraction ve, and plasma volume fraction vp. These are in turn used to estimate the concentration of chemotherapy drug in the tumour. The DW-MRI data return a measure of the apparent diffusion coefficient (ADC) of water in the tumour, used to estimate tumour volume fraction at each voxel. Initial parameters calculated in this manner from pre-treatment data are used to calibrate the model to data after one cycle of NACT. This returns three personalised coefficients (tumour cell proliferation rate, diffusion coefficient in the absence of stress, and drug efficacy) that are used in the model's forward evaluation.

We apply this process to data from patients from the CHERNAC clinical trial to predict their tumour response to NACT according to the model. Model outputs are compared to images acquired after three cycles of NACT.

Immersed-boundary variational methods: Theory, data structures, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NEW APPROACH FOR THE ENFORCEMENT OF NEUMANN BOUNDARY CONDITIONS WITH THE SHIFTED BOUNDARY METHOD

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ABSTRACT

Immersed/embedded boundary computational methods offer a useful alternative to traditional boundary conforming approaches, particularly in cases involving high geometric complexity. The trade off with standard embedded boundary methods (cutFEM, Finite Cell Method, etc.) is that they often require tedious cell cutting processes, specialized quadrature operations, and careful management of so called "small cut-cells". The Shifted Boundary Method (SBM) is an alternative approach that addresses the small cut-cell problem by eliminating the need to perform cell cutting altogether.

The SBM employs the use of surrogate domains which contain only fully formed elements by design (no cuts). The true boundary conditions are shifted onto the location of the surrogate boundary by way of field extension operators constructed with Taylor expansions, preserving accuracy. Indeed, if the boundary conditions from the true domain are assigned to the surrogate without proper modification, the resulting convergence will be sub optimal. Optimal convergence rates have been demonstrated for essential boundary conditions, where the solution and its gradient are readily accessible (in the case of piece-wise linear interpolation functions). However, shifting Neumann boundary conditions requires a modified approach since the higher order terms in the Taylor expansion are unavailable (all terms beyond first order derivatives are zero for linear elements).

Neumann boundary conditions are ubiquitous in many applications, particularly in solid mechanics problems with stress-free boundary conditions. The aim of this work is to provide an approach that achieves optimal convergence for shifted Neumann boundary conditions without the use of a mixed formulation, maintaining the same data structure requirements as the Dirichlet SBM boundary conditions. This is accomplished by introducing extension terms to the variational statement evaluated on the Neumann boundary, which account for the distance between the true and surrogate boundary. Additionally, special care is taken to maintain consistency within this formulation. We show how these implemented modifications provide a stable and accurate scheme for embedded Finite Element computation involving Neumann boundary conditions.

Immersed-boundary variational methods: Theory, data structures, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A GENERALIZED WEIGHTED SHIFTED BOUNDARY METHOD FOR PROBLEMS WITH EVOLVING DOMAINS

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ABSTRACT

Unfitted/Immersed or Embedded Finite Element methods have gained significant attention in the past decade for their effectiveness in simulating problems in complex geometries. However, many existing methods in the literature necessitate ad-hoc modifications of standard Finite Element data structures. This often involves tessellation of elements intersected by the embedded boundary, the construction of special quadrature rules, or the definition of geometry-dependent surrogate boundaries.

In this work, we propose a novel approach: a generalization of the Weighted Shifted Boundary method [1], which eliminates the need for special data structures or quadrature rules, and enables the solution of unfitted problems with geometry-independent Finite Element spaces. This newly introduced framework holds particular significance for problems involving evolving geometries and potential topological changes. Applications extend to scenarios such as topology optimization or fluid-structure interaction problems where the ability to handle dynamic geometries is crucial.

In this talk, we will present the formulation of the Generalized Weighted Shifted Boundary method and showcase its application to a variety of problems with evolving domains.

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Architected materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREDICTING THE DOMAIN OF LINEAR ELASTICITY OF ARCHITECTED MATERIALS - FOCUS ON SYMMETRIES

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ABSTRACT

Introduction
Modern engineering challenges have pushed forward the use of architected materials and called for a new branch of material science to be explored. These special materials exhibit unconventional properties directly linked to their geometry. When composed of slender elements, architected materials can undergo large deformations exhibiting geometric non-linearities through buckling or snapping behaviors of the cell walls. Furthermore, as any conventional material, their constitutive material could enter its non-linear domain. The combination if these two limits define the domain of linear elasticity of the architected material. This presentation will present the domains of linear elasticity of various 2D architected materials and relate the symmetry of the domain to that of the parent material.

Method
The domain of linear elasticity is constructed from the intersection of the non-buckling domain of the architected material and the linear elasticity domain of its constitutive material. It is well-known that buckling in architected materials can happen at different scales, especially when working with periodic architected materials. Bloch-wave analysis is the appropriate tool for predicting buckling in such periodic materials. This presentation will only consider 2D lattice periodic architected materials composed of beam elements that are modelled with Euler-Bernoulli beam theory. Moreover, the method only accounts for isotropic constitutive material and constant cross-section beams but the latter limitation can be lifted. The method could be extended to architected materials composed of plate or shell elements.

Results
The method has been validated on the classical examples of regular square, triangular and hexagonal honeycombs. The observed bifurcated patterns presented in the literature both numerically and experimentally are predicted by our method and results on the shape of the non-buckling domain can be retrieved.
More interestingly, it is possible to correlate the shape of the domain of linear elasticity with the symmetry of the parent architected materials. Based on several examples, it is observed that the symmetry group of the architected material is partially transferred to the symmetry group of the domain of linear elasticity, when observed in the deviatoric space. This can be explained by a tensorial representation of that domain.

Physics-based data-driven modeling and uncertainty quantification in computational materials science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE UNCERTAINTY QUANTIFICATION AND PROPAGATION FOR COMPOSITE MATERIALS SYSTEM WITH AGGLOMERATION AND STRUCTURAL ANOMALIES

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ABSTRACT

Although advancements in manufacturing technologies have enabled material design optimization at multiple scales, the microstructure anomalies and uncertainties present at each scale have not been considered comprehensively enough for them to be robust to manufacturing variations. Specifically, the agglomerations, formed due to high surface energy and attractive Van der Waals forces between nanoparticles in the microscale, as well as voids forming due to different processing conditions at the mesoscale, significantly impact the mechanical properties of the composite materials at higher scales [1,2]. Consequently, considering these anomalies at various length scales of the material's structure and understanding their uncertain effects on a part's response are crucial for designing engineered parts that are robust to various sources of uncertainty.

To account for these anomalies, an efficient bottom-up uncertainty quantification and propagation framework bridging the microscale and the mesoscale to establish a design allowable range for the composite material system at the part-scale is presented. At the microscale, the agglomerated material system is characterized and reconstructed from a few (approximately 30) experimental images and reinforced with interphase percolation for property enhancement. At mesoscale, varying bead structures are created to reconstruct interlayer voids. Subsequently, a copula-based sampling strategy that offers significant dimension reduction to preserve key information across multi-scale design space with a mechanistic reduced-order model that enables fast property prediction to create an efficient uncertainty quantification and propagation framework. The framework provides further understanding regarding the influence of anomalies at lower scales on the part-scale performance. Finally, the applicability of the framework is demonstrated for an additively manufactured polymeric material system, highlighting the importance of considering the effects of process-induced microstructure features on the part performance.

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Advances in multi-scale, multi-material, and multi-component Topology Optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STRUCTURAL MULTI-MATERIAL DESIGN AT DIFFERENT LENGTH-SCALES USING TOPOLOGY OPTIMIZATION

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ABSTRACT

In recent years, substantial efforts have been made in the development of Topology Optimization (TO) procedures for a more sustainable technological advancement. One of these efforts consists in the design of multi-material structures. In fact, conventional materials used in the past may not be able to fulfil today's design objectives and requirements. This motivates to enlarge the design space to include multi-material solutions in structural design at different length-scales. Multi-material design can lead to more efficient structures in terms of stiffness and/or strength, while also allows for tailored mechanical and thermal behaviours, such as negative indexes on mechanical and thermal properties. Many industrial sectors, ranging from aerospace to biomechanics fields, could benefit from the use of non-conventional materials, although their fabrication still remains a challenge.

This work addresses Multi-Material Topology Optimization (MMTO) applied to specific cases of practical interest. Firstly, one explores the potential of multi-material design to improve the efficiency of structures at different length-scales [1]. Two different problem formulations can be stated: (1) compliance minimization, and (2) stress minimization. Both problems can be solved at the microscale and macroscale, either independently or in a concurrently manner (multi-scale). Regarding the stress minimization problem, two types of design solutions can be considered. On one hand, two solids coexist being bonded together across sharp interfaces. On the other hand, a Functionally Graded Material (FGM) is obtained as an extensive smooth variation of material properties on account of varying composition’s volume fractions of both solids throughout the design domain, such that a more evenly stress distribution is attained. Lastly, Asymptotic Homogenization (AH) techniques, along with MMTO, are used to design optimal porous composite materials consisting of a periodic microstructure, so-called metamaterials. These metamaterials aim for negative indexes on mechanical and thermal properties, such as negative Poisson’s ratio and/or negative Coefficient of Thermal Expansion (CTE). The AH theory assumes periodicity at the microscale, that it is infinitesimally small in comparison to the macroscale. However, in practice the composite material will only encompass a finite number of repetitions. To assess the feasibility of optimal metamaterials in engineering practice, it is crucial to investigate the proximity of the equivalent thermoelastic properties predicted by the AH to those exhibited by real composites.

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Mathematics and algorithms for predictive digital twins (DT)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MULTIRATE INTEGRATION FRAMEWORK APPLIED TO SOLID-SOLID AND FLUID-FLUID INTERACTION MODELS

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ABSTRACT

We discuss a framework for multirate integration of multi-component systems with coupling across interfaces. The problem is to derive algorithms that support different time step sizes for each component. In the context of multirate coupling, there can be problems with accuracy, stability, or preservation of properties such as system invariants. The proposed framework provides a way to derive algorithms with the desired properties. The multirate coupling is based on the recent work (Connors and Sockwell, 2022) that treats the subdomain integrators as piecewise polynomial in time using the mathematics of discontinuous-Galerkin-in-time methods. These piecewise representations are then mapped into a smooth coupling space that spans some predefined interval of time called a "coupling window". Two example applications are discussed: solid-solid interaction and a two-layer air-sea proxy using rotating thermal shallow water equations. We show how to apply the framework and customize the multirate coupling for each application. Numerical examples illustrate the accuracy, stability and preservation of a system invariant with different time step sizes for each component.

Computational methods in environmental fluid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ASSESSING ATOLL ISLANDS' VULNERABILITY UNDER CLIMATE CHANGE CONDITIONS

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ABSTRACT

Atoll islands are home to tens of thousands of people from the Maldives, Tuvalu, Kiribati, the Marshall Islands, and several other countries. However, it has been established that many of them will become uninhabitable during the 21st century due to climate change (1). Sea level rise (SLR) is expected to be the most significant threat due to their low elevation and limited area, resulting in more frequent and extensive inundations, groundwater salinity intrusions, and chronic coastal erosion.
Up-to-date studies have improved the understanding of long-term sea level variations using sparsely distributed observations and satellite data (2), limiting the applicability to future conditions. Efforts in numerical modeling have focused on combining SLR and waves, but primarily through parametrization and for small sets of islands (3), due to the high computational costs of combining large-scale ocean dynamics with small-scale wave impact on the islands' coastlines.
Thus, our objective is to improve the understanding of the evolution of atoll islands' coastline and their inundation risk in a changing climate. Through numerical simulations, we integrated the effect of the ocean hydrodynamics, weather, waves, and sea level rise to represent past, present, and future conditions. We used ADCIRC+SWAN to represent the hydrodynamics of the Pacific, with the primary interest in the Marshall Islands. For the historical period, we forced the model with atmospheric conditions from ECMWF Reanalysis 5 (ERA5). We used the climate and SLR predictions from the WCRP Coupled Model Intercomparison Project (CMIP) multimodel mean under the SSP245 scenario for future scenarios. We assessed variations in potential inundation over time and shifts in flood frequency, characterizing the magnitude, time frame, and variability of the impact that different islands will experience, as well as wave power and, hence, the erosion risk. All this information is crucial for decision-makers in order to plan adaptation measurements that allow to preserve the habitability of these islands.

Storlazzi, C., Elias, E. & Berkowitz, P. Many Atolls May be Uninhabitable Within Decades Due to Climate Change. Sci Rep 5, 14546 (2015). https://doi.org/10.1038/srep14546
Murray R. Ford, Paul S. Kench. Multi-decadal shoreline changes in response to sea level rise in the Marshall Islands. Anthropocene 11, 14-24 (2015). https://doi.org/10.1016/j.ancene.2015.11.002
Amores, A., Marcos, M., Le Cozannet, G. et al. Coastal flooding and mean sea-level rise allowances in atoll island. Sci Rep 12, 1281 (2022). https://doi.org/10.1038/s41598-022-05329-1

VIBROACOUSTIC BANDGAP MAXIMIZATION THROUGH TOPOLOGY OPTIMIZATION

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ABSTRACT

The control of wave propagation through metamaterials is extensively researched in different disciplines. In the field of noise and vibration, metamaterials are mostly designed to obtain bandgaps, i.e. frequency ranges without free wave propagation. The unit cell designs commonly target the attenuation of structural or acoustic waves separately. Only more recently, metamaterial designs have come forward which have extraordinary performance characteristics by obtaining a simultaneous acoustic and structural bandgap, e.g. [1]. To result in this simultaneous bandgap, intricate complex unit cell geometries are required which are difficult to tune and require expert knowledge since both the elastic and acoustic phase is of importance and influence each other. Moreover, commonly one of the bandgaps is narrow banded. In this regard, optimization routines can be an important enabler to automate the design of these novel vibroacoustic metamaterials. In this work, a 2D topology optimization routine is presented with the objective of maximizing the vibroacoustic bandgap of the in-plane wave modes. During optimization, the vibroacoustic coupling in the design and dispersion curves is considered. A volume constraint is included to control the light-weight character of the designs. Additionally, a connectivity constraint is required to avoid material islands and control the stiffness of the obtained designs. With this framework, novel vibroacoustic metamaterial unit cell designs are obtained, which present wide omni-directional simultaneous acoustic and elastic bandgaps. Moreover, the trade-off between stiffness, weight and attenuation performance during the design of vibroacoustic metamaterials is investigated.

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ADAPTIVE COVARIANCE ESTIMATION FOR MULTI-FIDELITY OPTIMIZATION

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ABSTRACT

Multi-fidelity variance-reduction techniques (e.g., approximate control variates [1] and multilevel BLUEs [2]) have seen considerable attention in recent years, in many cases providing orders-of-magnitude computational savings in accurately estimating statistics of a high-fidelity model. These methods require the covariance matrix across model fidelities, which is usually estimated via pilot sampling or reinforcement-learning techniques [3] in conjunction with the sample covariance formula. Depending on the model ensemble available, this covariance estimation can be costly or inaccurate, leading to suboptimal estimators. Furthermore, most multi-fidelity estimators are not designed with an outer design optimization loop in mind, where covariance information and thus optimal estimator properties may vary substantially from design to design. In this work, we leverage uncertainty information in a parameterization of the covariance matrix to adaptively guide pilot sampling simultaneously as the outer optimization loop converges. In doing so, the overall multi-fidelity optimization process can converge more efficiently. We demonstrate this through applications for multi-fidelity optimal experimental design.

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Recent advances in high-order methods for computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

METRIC-BASED CURVED MESH ADAPTATION USING HIGH-ORDER EDGE OPERATIONS

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ABSTRACT

We present a strategy for adapting high-order curved unstructured meshes using local mesh modification operations to conform to a prescribed metric field. Curved meshes are required for high-order discretizations, but they are difficult to generate and adapt, especially when anisotropic elements are required near curved boundaries. Typically, mesh adaptation is performed by first converting the curved mesh to a linear mesh, adapting the linear mesh, and re-curving the linear mesh around curved boundaries. The re-curving process can be done through solving an optimization problem or an analogous physics based elasticity problem. However, these approaches are computationally expensive and do not guarantee a valid curved mesh. To address this problem, we extend traditional linear edge-based mesh modification to high-order elements. The use of a sequence of individual local operators guarantees that the high-order mesh remains valid and represents the curved geometry throughout the adaptation process as any modification that leads to invalid elements is rejected. Results for two-dimensional adaptive simulation for a variety of mach and Reynolds numbers are presented. Comparisons with global linear re-meshing with re-curving show similar output error convergence, similar computational cost as re-curving, and improved robustness.

Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A 1D HYBRID BEAM-SHELL TUBE MODEL FOR PROGRESSIVE CRACKS IN PIPELINES

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ABSTRACT

The industrial energy sector oversees an extensive quantity of pipelines, and their behavior under normal operation or incidental event shall be understood. Recent works have focused on simulating such pipe structures under intense dynamic loading . However, under the context of the utmost safety of nuclear power plants, it is imperative to investigate extreme accidental scenarios. As a consequence, pipe deformations, as well as hypothetical pipe ruptures, have to be examined.

An advanced tube model has been previously developed in [1] as an uniaxial enriched beam model for thin-walled pipes. It combines a beam and a shell behavior to model the pipe cross-section deformation with Euler-Bernoulli and Love-Kirchhoff hypotheses, respectively. The displacement fields are expanded as Fourier series with respect to the angular parameter, and the degrees of freedom of the model correspond to the Fourier coefficients.

This new mechanical pipe behavior model was formulated within a fast transient time-explicit and Lagrangian Finite-Element framework. Comparisons with multi-dimensional FE models were also performed in [1] to validate the static and dynamic behavior of the advanced pipe model.

In this work, the hybrid shell-beam pipe element is completed in order to study the evolution of a progressive crack through the pipeline. For this purpose, new degrees of freedom are added to allow dynamic crack propagation along the pipe. A short presentation of the kinematics required to accurately represent pipe cracking behavior is conducted. The proposed model is then examined through simple examples of straight pipe or elbow under various loadings, such as internal pressure and flexion. The results and quantities of interest, such as crack speed and position, are compared with a 3D erosion model as in [2] in the explicit dynamics framework to assess the physical reliability of the 1D model.

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Multiphysics and data-driven modeling for cardiovascular biomedicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFECTS OF BICUSPID AORTIC VALVE MORPHOLOGY ON HEMODYNAMICS IN THE ASCENDING AORTA

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ABSTRACT

A bicuspid aortic valve (BAV) is a common congenital cardiac disorder where the aortic valve only has two cusps instead of the typical three and is linked to aortic valve dysfunction and aortic aneurysm and affects approximately 1.4% of the population [1]. There are three major types of morphologies that BAVs present in, 90% of which are type 1 valves, where two of the three leaflets are fused. Additionally, several studies have shown a significant variation in BAV morphology within type one BAVs. One study defined variations of type one BAVs based on which two leaflet cusps were fused and whether they were completely or partially fused [2]. This study simulated and analyzed six type 1 BAV morphologies using a validated open-source computational fluid-structure interaction framework based on immersogeometric analysis [3]. Immersogeometric analysis is a computational technique that immerses designs geometries in a non-conforming mesh. This method allows the simulation of flow past complex geometries without worrying about how a boundary-fitted mesh will deform, especially for thin structures such as valve leaflets. To more accurately model the diseased BAVs, both the aortic leaflets and wall employ hyperelastic soft tissue materials and population-based geometric models. Using the above methods, we can isolate the impact of the different valve morphologies on hemodynamics in a physiologically realistic blood flow model. Key metrics for each morphology were studied, such as the wall shear stress in the ascending aorta, valve regurgitation, and valve stenosis. Despite the prevalence of BAVs, the hemodynamics due to varied BAV morphologies are understudied, and tools to assess which BAV patients are most at risk are not readily available. Our open-source computational FSI framework provides a practical approach to investigate these valve morphologies which can later be extended to patient-specific models to increase patient health outcomes.

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Computational damage and fracture mechanics
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A SYSTEMATIC METAMODELING FRAMEWORK FOR OPTIMIZING ENERGY ABSORPTION STRUCTURES SUBJECTED TO LOCALIZED DAMAGE

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ABSTRACT

The use of optimization algorithms in designing energy absorption structures has become popular due to their ability to determine the optimal size of geometric features, maximizing performance relative to weight. This approach is particularly valuable in industries where weight reduction is crucial, such as aerospace and automotive. With the advent of digital design and advances in 3D printing technology, optimization can now explore configurations that were previously difficult or impossible to manufacture.
In structures such as composite metallic sandwiches damage modeling is essential to accurately represent the penetration and perforation process when subjected to high velocity impact. These structures can also experience delamination effects, where the thin face sheets separate from the cellular core. The adhesive bonding the components is also susceptible to damage. By considering damage for each component and the adhesive, engineers can better understand the behavior of the structure under impact and make informed design decisions to enhance its energy absorption capacity and structural integrity.
However, this process can be computationally intensive. The proposed metamodeling framework aims to mitigate the computational cost impact in the optimization of structures subjected to high velocity impact. By using a parameterized finite element model of a 3D sandwich structure and space filling Design of Experiment (DOE) techniques for defining sampling points, the framework seeks to create an Artificial Neural Networks (ANN) metamodel that can approximate the behavior and performance of the structure. ANN are then used in combination with genetic algorithms to find the optimum set of variables that improve the energy absorption capacity of the structure.
This metamodeling approach offers several benefits. First, it reduces the computational cost associated with explicitly solving highly non-linear finite element models with damage. Second, it allows for efficient exploration of a wide range of design variables, enabling the discovery of novel configurations that maximize energy absorption. Finally, it provides a systematic framework for optimization that can be applied to various types of energy absorption structures, facilitating design innovation and efficiency.

AN IN SILICO APPROACH FOR SAFETY PHARMACOLOGY STUDIES ON VASCULAR TISSUE

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ABSTRACT

This work is devoted to the development of in silico models aimed at predicting the effects of drugs on vascular vessels. Specifically, a mathematical model is proposed to reproduce the experimental data of the ROTSAC (Rodent Oscillatory Tension Set-Up used for studying Arterial Compliance) setup [1]. Furthermore, the following two hypotheses on the mechanical impact of vasoconstrictors and vasodilators are investigated numerically: (i) the compound exclusively affects the smooth muscle cells (SMCs) of the vessel; (ii) the compound can alter the stiffness of the endothelium. The arterial wall is modelled as a hyperelastic 3D shell (Ogden law) [2] reinforced with active fibers characterized by an affine stress-strain constitutive law with two parameters: the pre-stress and the elastic modulus of the fibers (see [3]). The inputs of the model are the force measured in the experiment and the parameters describing the behaviour of the material (Young modulus, Poisson ratio, active pre-stress and elastic modulus, initial length, width and thickness of the aortic segment). Parameter estimation is performed with a CRS2 optimization algorithm with local mutation. The numerical results indicate that there are not significant variations in the Young modulus for vasoconstrictors or vasodilators compared to the baseline. However, the most substantial impact is observed on the parameters of the smooth muscle cells' fibers, particularly the active pre-stress and elastic modulus.

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Advances in computational biomechanics and mechanobiology
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POROELASTIC MODEL OF FLUID EXCHANGE BETWEEN BRAIN AND SUBARACHNOID SPACE: A FINITE ELEMENT IMPLEMENTATION WITH JUMP CONDITIONS

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ABSTRACT

The brain, which is suspended in cerebrospinal fluid (CSF) but not attached to skeletal muscles, moves within the skull. The origin and physiological impact of this movement are yet to be understood, but we suspect that it may substantially contribute to CSF circulation and clearing of toxic metabolites from the central nervous system (CNS). Here we present an initial investigation of how mechanical stimuli can be transmitted to the CNS and cause fluid exchange between brain and the surrounding subarachnoid space (SAS). We adopt a large-strain poroelasticity model based on mixture theory with incompressible constituents: a hyperelastic solid, and a fluid moving according to a Darcy flow model. This model was implemented via an arbitrary Lagrangian–Eulerian finite element method (FEM). Both brain and SAS were treated as poroelastic (the SAS is trabeculated and has some load-bearing properties), but with different transport and mechanical properties. Both pressure and fluid velocity are discontinuous across the brain/SAS interface. We performed simple simulations of how the CNS moves in response to mechanical stimuli provided by the vertebral venous plexus (VVP), a network of veins that can communicate pressure changes from the thoracic cavity to the dura of the spinal cord. While our geometry is highly simplified, our results are encouragingly in line with experiments. To obtain these results we had to overcome significant numerical challenges arising from (i) the enforcement of the constituents' incompressibility condition (yielding a nontraditional inf-sup condition), and (ii) the enforcement of the jump conditions at the brain/SAS interface. Particularly challenging was the identification of stable FEM spaces. Here, we will review the jump conditions that arise naturally from the mass and momentum balance laws. We will then discuss our implementation by way of integration by parts for the mass balance equation but not the momentum equation. Our implementation is nontraditional and it explores the use of unusual FEM stable spaces in that the pressure field was interpolated by linear and quadratic Lagrange polynomials with a discontinuity at the brain/SAS interface, whereas the fluid velocity field was interpolated via discontinuous Lagrange polynomials within both the brain and SAS domains. These FEM spaces appear to be inherently stable. We found difficulties in identifying stable spaces with globally continuous (except at the interface) interpolations for both pressure and velocity. However, we also found that stabilization following a Virtual Multi-Scale approach yields promising results.

Emerging frontiers and methods in digital manufacturing: Modeling, simulation, and beyond
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A COSSERAT FINITE ELEMENT MODEL FOR DEFORMATIONAL BEHAVIOUR OF UNCURED FIBROUS COMPOSITES DURING PROCESSING

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ABSTRACT

Composite materials, known for their high stiffness and strength-to-weight ratio, are highly sought after in various industries such as aerospace, automotive, and sporting goods. During manufacturing, fibrous layers, known as plies, are precisely aligned and stacked to achieve desired performance characteristics. However, the layered and soft nature of raw composite materials poses significant challenges, including risks of ply shearing, slipping, or wrinkling, as they are transformed into structural parts.
This research addresses the simulation challenges of layered composite materials. Unlike traditional forming software such as Aniform and PAM-FORM, which model each layer separately, this study employs the Cosserat continuum (micropolar) theory to homogenize the layered kinematics. This approach effectively captures asymmetric shear and intrinsic bending behaviors. A special purpose explicit finite element model, developed in MATLAB, employs high-order elements and a co-rotational approach to enable accurate material orientation tracking. The model effectively handles the large deformation and strain typically experienced by the soft and compliant composite material during its pre-curing stages of processing.
The model's effectiveness is validated through comparisons with experimental data and existing computational models based on classical continuum mechanics. This includes deformation simulations of frictionless thick paper stacks [1] and plastic sheets stacks with interlayer friction [2].
For a direct application in composite manufacturing, the model is shown to capture wrinkle formation in composites during corner consolidation [3]. It is found that such factors as ply bending stiffness and the inter-layer friction coefficient play influential roles in determining the frequency and size of wrinkles.
This research is the first to implement a Cosserat continuum model within an explicit framework for composite processing. While others have used the Cosserat continuum, the current computational framework is particularly effective and robust for handling the large deformation of soft, layered, fibrous materials.

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Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A HIGH-FIDELITY THERMAL-FLUID-SOLID MODELING APPROACH TO UNDERSTAND DEFECT FORMATION AND RESIDUAL STRESSES IN ADDITIVE MANUFACTURING BUILDS

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ABSTRACT

Qualification of additively manufactured (AM) components for high consequence engineering environments requires science-based understanding of AM processes. Computational simulation has been established as an effective means of probing the complex physics that occur during AM. Defects such as voids, or pores, can be formed as a result of changes in direction of the laser path, or incorrect laser parameters resulting in potentially defective builds. This work uses a one-way coupled thermal-fluid-solid analysis workflow to predict residual stresses and post-build material properties in the presence of voids formed during laser melting and AM processing. Initially a thermal-fluid modeling approach is used to predict laser interactions, deposition patterns, temperature distributions, fluid flow in the melt pool, and the formation of a pore. Results from this thermal-model are then pushed forward into a solid mechanics simulation framework to predict solid phase stresses and the resulting material properties. This talk will show several examples of laser scans patterns that result in pore formation in titanium and aluminum alloys. This modeling approach provides a high-fidelity multiphysics solution for AM processes, albeit at a severe computational cost. These results are useful in quantifying the effects of defects in AM components with the inclusion of residual stresses on structural performance for high consequence engineering environments.

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REDUCED BASIS STABILIZATION AND POST-PROCESSING FOR THE VIRTUAL ELEMENT METHOD

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ABSTRACT

Virtual element methods are known to tackle complex geometries without limitations on the degree of the polynomial that partially contributes to the approximate solution. An important aspect of this method is that we are not required to explicitly compute the basis functions of the VEM space since these are solutions of PDEs. Due to this fact, several quantities are not computed exactly. Two of these are the bilinear form, for which the action on the nonpolynomial part is handled by a stabilization term, and the error, where the contribution of the nonpolynomial part is neglected.
We propose a model order reduction technique constructed by means of the reduced basis method (RB) for efficiently solving the equation associated to each virtual basis function. The idea is to replace the stabilization term with an actual approximation of the nonpolynomial contribution. We show that this operation produces good results even if done in a very rough way. This novel approach improves the convergence properties of VEM when applied, for instance, to anisotropic second order diffusion equations, when standard stabilization recipes show poor performance.
In post-processing framework, it is well known that, when a PDE is solved with VEM, the degrees of freedom of the discrete solution allow only the computation of projections onto discontinuous polynomial spaces, so that the solution is not conforming. The RB approximation of the virtual functions can also be exploited for reconstructing conforming solution in the VEM space. This task can be useful to carry out operations such as visualization, reconstruction in subdomains, pointwise evaluation and evaluation of the conforming error when benchmarking the method.

Fabio Credali, Silvia Bertoluzza, and Daniele Prada. "Reduced basis stabilization and post-processing for the virtual element method." Computer Methods in Applied Mechanics and Engineering 420 (2024): 116693.

Emerging frontiers and methods in digital manufacturing: Modeling, simulation, and beyond
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A PARTICLE FINITE ELEMENT METHOD FOR THE SIMULATION OF 3D CONCRETE PRINTING

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ABSTRACT

Over the past few decades, 3D concrete printing (3DCP) has led to significant developments in building design and construction. This technology employs a digitally controlled robotic arm to deposit cementitious mortar filaments, aiming to create arbitrary-shaped items and structural elements. The potential benefits of 3DCP are manifold, including the rapid construction of free-form designs without traditional formwork, decreased reliance on human labour, reduced building costs, and shorter construction times.

However, for the widespread adoption of 3DCP, several challenges need to be solved at both practical and numerical levels. Specifically, the development of efficient and accurate computational tools is crucial for enhancing understanding of the printing process and predicting outcomes in terms of material, structural, and process performance. In this contribution, we simulate the printing process of cementitious materials using a single-phase fluid model [1]. The fluid's motion is governed by Lagrangian Navier-Stokes equations with a non-Newtonian rheological law to describe the material behaviour. To handle numerically large displacements and nonlinearities, the Particle Finite Element Method (PFEM) is here employed [2]. The unique capabilities of PFEM address various numerical issues, including precise treatment of inter-layer contact and the imposition of time-dependent moving boundary conditions at the nozzle outlet [3].

The model has been validated using experimental data from different printing scenarios, providing insightful information on the printing process that perfectly aligns with experimental results. The proposed model can be used as a tool for evaluating the extrudability of cementitious mixes based on rheological parameters. It will be a valuable support to experimental campaigns for developing new cementitious inks, optimizing printing parameters, and predicting occurrences of plasticity and buckling failures during the printing of arbitrarily shaped objects.

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Advances and applications of polytopal methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A HYBRID HIGH-ORDER METHOD FOR PHASE-FIELD MODELING OF FRACTURE PROPAGATION

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ABSTRACT

In this work we develop and investigate a Hybrid High Order method (HHO) for the problem of modeling of fracture propagation. The formulation of the model exploits a phase-field approach for fracture modeling, which has the advantage of being a continuous method that integrates naturally with Continuous Media Mechanics.

HHO methods offer several advantages with respect to traditional numerical schemes; in particular they support general meshes with non-matching interfaces and arbitrary approximation orders. A direct consequence is the ability to support non-conforming adaptivity of the mesh, which makes HHO methods particularly suited to the case of physical phenomena occurring in small areas of the domain such as fractures propagation.

We exploit the open source HArD::Core library which was developed by D. Di Pietro and J. Droniou and implements HHO schemes for 2D and 3D applications. The library has already been applied to physical problems but not yet to fracture propagation. Thus, we propose to extend it to fracture problems with a novel HHO method based on a coupled system for displacement and phase-field variable in two space dimensions.
Numerical validation on model test problems is also provided.

Fluid-structure interaction: Methods and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL SIMULATION OF FLUID-STRUCTURE INTERACTION WITH MANY RIGID BODIES

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ABSTRACT

A methodology for the simulation of many rigid bodies (RBs) colliding between them and with the walls, and interacting with a Newtonian fluid is presented. The RBs are simulated with the "prtclsys" C++ library, which represents RBs as a set of 4 or more particles with restrictions between them, and uses quaternions for internal computations. The bilateral restrictions are considered via iterative penalization, whereas unilateral restrictions (e.g. collisions between the RBs themselves and with the walls) are computed via penalization. Interaction between the RBs and the fluid is computed via an embedded technique. The Approximate Nearest Neighbor Tree algorithm is used to determine if a given fluid cell belongs to an RB or not to compute the penalization terms, and hence the force of the RB. Regarding the structure, the "prtclsys" library allows the simulation of relatively complex arrays of rigid bodies, links, moors, contacts of the bodies with surfaces, and other restrictions. All items in the simulation are represented as particles, including the rigid bodies which are represented as arrays of four or more particles arranged such that they have the same mass and inertia moments as the target body. The distances between the particles in the rigid body are fixed using restrictions, and the whole dynamic of the system is solved as a system of differential-algebraic equations.

SPATIAL NEURAL ODES FOR MODELING BLOOD FLOW IN STENOSED ARTERIES WITH DEFORMABLE WALLS

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ABSTRACT

Coupled partial differential equations serve as a fundamental framework for describing a wide range of multi-physics phenomena in the natural world. Notably, cardiovascular flows exemplify the complex interplay of these equations, carrying significant real-world implications. Yet, accurately and efficiently modeling such phenomena poses considerable challenges. Here, we tackle the problem of blood flow in a stenosed artery with deformable walls, where the geometry is idealized but the problem is made reasonably complex by a realistic pulsatile inlet flow rate waveform and fluid-structure interaction (FSI). We create a low-dimensional model based on neural ordinary differential equations (neural ODEs) [1], inspired by the 1D blood flow equations. Neural ODEs have been proven to be a versatile tool for scientific machine learning and fluid flow modeling. Data-driven approaches have shown promising results in the past for cardiovascular applications [2], but neural ODEs have not yet been leveraged for blood flow problems. However, solving a coupled set of PDEs poses further challenges that have rarely been addressed in the literature. The solution of one PDE has to be fed into the other PDE, which requires solution smoothness and stability. We demonstrate that in 1D transport problems with periodic boundary conditions in time, a reformulation of neural ODEs in space instead of the traditional temporal formulation, shows significant improvement in the stability of the trained coupled PDEs and their extrapolation accuracy with respect to different inlet boundary conditions. Casting the neural ODEs in space, rather than time, is shown to overcome two main challenges. First, it makes it easy to use different inlet boundary conditions as they are transformed to initial conditions in the spatial neural ODE model. Second, it provides accurate derivatives in the spatial direction, enabling coupling with the continuity equation. This innovative framework accurately captures flow rate and area variations, even when extrapolating to unseen inlet flow rate waveforms. The promising results from this approach offer a different perspective on deploying neural ODEs to model coupled PDEs with unsteady boundary conditions, and could be applied to other unsteady transport problems far beyond cardiovascular flows.

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Physical models and reduced order models augmentation with data for physics-informed machine learning in real-world applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ON THE ROLE OF THERMODYNAMICS AS INDUCTIVE BIAS FOR LEARNED SIMULATORS

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ABSTRACT

We review how thermodynamics can act as a very effective inductive bias when developing learned simulators based on the employ of deep learning.

To impose the fulfillment of the first and second principles of thermodynamics, we assume that the evolution of the system has a metriplectic structure (i.e., a combination of symplectic and metric forms). The symplectic structure ensures the conservation of energy in closed systems, while the metric part imposes a no-negative entropy production.

In combination with geometric biases (through the use of graph neural networks), the resulting approach gives very promising results, showing to be very robust for out-of-distribution situations.

Examples are provided that show the potential of the suggested method.

Multiscale methods for advanced manufactured materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-PHYSICS DRIVEN THREE-SCALE APPROACH FOR ULTRA-FAST RESIN TRANSFER MOLDING (UF-RTM)

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ABSTRACT

We introduce an efficient computational framework designed for simulating the mold filling process in ultra-fast resin transfer molding (UF-RTM), a term used to describe the application of ultra-low viscosity resins (50-200 at room temperature) under ultra-high pressure (~200 bars)—a combination of pressure and viscosity not yet explored in practical applications. The primary innovation of this framework is its data-physics driven nonlinear homogenization method. This approach effectively tackles the unique challenges posed by this high-pressure, low-viscosity scenario while circumventing the extensive computational demands usually needed for simulating intricate microstructures at multiple scales. The proposed data-physics driven mold filling model has been verified against the direct numerical solutions of the Navier-Stokes/Brinkman equations. Furthermore, we introduce a cost-effective tow saturation model, which has been trained to a high-fidelity method based on the numerical solution of the Cahn-Hillard phase field model with Stokes equations at the pore level. This framework shows promise for ultra-fast manufacturing processes of composite parts, contributing to improvements in mold design, reduction of void formation, and consequently leading to rapid development time and minimized production waste.

Advanced model order reduction techniques for computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

REDUCED ORDER AERODYNAMIC MODELING RESEARCH FOR HIGH-PRESSURE CAPTURING WING CONFIGURATIONS BASED ON PROPER ORTHOGONAL DECOMPOSITION AND SURROGATE METHOD

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ABSTRACT

Fast aerodynamic prediction is one of the key technologies for the multi-disciplinary optimization design of hypersonic vehicles. Most of the research focuses on vehicles with a single lift surface, such as blended-wing-body and waverider configurations. However, if there are strong aerodynamic interactions between the various components of a vehicle, the conventional prediction method may be challenging to be effective. Recently, a novel hypersonic aerodynamic configuration, called high-pressure capturing wing (HCW) [1], has been proposed to achieve the goal that a vehicle with a large volumetric ratio can simultaneously have a high lift-to-drag ratio and a high lift coefficient, which has been demonstrated by the hypersonic experimental investigation referred in [2]. For this configuration, a shock wave induced by the fuselage strongly interacts with the HCW. Therefore, the engineering estimation of aerodynamic forces for the HCW encounters difficulties. Aimed at solving the shortcomings of engineering estimation and computational fluid dynamics (CFD) calculation, a reduced order modeling (ROM) framework based on proper orthogonal decomposition (POD) and surrogate method is proposed. First, five parameters (the incoming Mach number, half-cone angle of body head, expansion angle of rear body, setting angle of HCW, and setting height of HCW) were set to the design variables in this study, and the uniform experimental design method was performed to obtain the 81 samples, uniformly distributed throughout the design space. Next, a CFD solver was used to evaluate the flow field characteristics of all the samples by solving the three-dimensional Reynolds-averaged Navier-Stokes (RANS) equations. Subsequently, a POD analysis process was performed for the pressure distributions acting on the HCW lower surfaces, and the Kriging method was used to establish the relationship between the five design variables and each POD basis mode coefficient. Test results indicate that the mean relative errors of pressure for all test samples can be less than 3%. Using more POD basis modes would not obviously improve the estimation accuracy when the basis modes reach 15. In brief, the reduced order modeling for the aerodynamic prediction of HCW configurations has good accuracy and efficiency.

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Computational particle-based solvers for multiphysics & multiscale simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MULTIPHASE SPH SOLVER FOR IN-FLIGHT SUPERCOOLED LARGE DROPLET IMPINGEMENT AND SOLIDIFICATION

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ABSTRACT

Supercooled large droplets (SLD) solidification is a complex multi-physics process of great importance for assessing in-flight icing problems. This work presents a multiphase smoothed particle hydrodynamics (SPH) solver that can conduct “numerical experiments” of SLD impingement and solidification under flight conditions.

In the present multiphase SPH solver, the momentum and energy equations are solved for flow and heat transfer, along with an equation of state linking pressure and density. A multiphase model is used to represent interfacial flows and a fixed ghost particle method to enforce boundary conditions. Artificial viscous and diffusive terms are employed to smooth physical fields and decrease numerical instability, while a particle shifting technique is used to alleviate anisotropic particle distribution. Several numerical techniques are proposed to model the complex physics of SLD impingement such as a contact angle model to represent the non-wetting properties of hydrophobic surfaces, a latent heat model to account for phase change, and a dendritic freezing model to capture dendrites growth in supercooled solidification.

The solver is validated against a series of experimental results, showing good agreement. It is then first applied to droplets impinging at flight speeds on a water film to study the effects on the post-impact water crown of droplet speed and diameter, water film thickness, and impact angle. Droplets impacting cold solid surfaces are then simulated to study freezing time and post-impact ice particle distribution for a range of speeds and impact angles. Following this, an improved contact angle model is used to study the interaction between droplets and hydrophobic/superhydrophobic coatings. Finally, SLD impingement on ice surfaces is studied via a dendritic freezing model, assessing supercooling degree and impact speed effects on residual ice.

This solver is a comprehensive toolset for the parametric study of SLD impingement and paves the way for an SLD icing simulation model more specifically applicable to aircraft flight speeds.

Computational mechanics of soft matter and machines
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN ANALYTICAL SENSITIVITY ANALYSIS FOR THE TOPOLOGY OPTIMIZATION OF HYPERELASTIC MATERIALS

Yi Cui[*1], Toru Takahashi[1] and Toshiro Matsumoto[1]*

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ABSTRACT

Topology optimization finds diverse applications across aerospace, mechanical, bio-chemical, and civil engineering disciplines. In most previous topology optimization studies, elastic materials (linear materials) were usually assumed when analyzing the displacement field. Hyperelastic materials, exemplified by for example Mooney–Rivlin Material, typically manifest a highly nonlinear stress-strain relationship, often undergoing substantial reversible strains. Addressing the complex topological optimization challenges of Mooney–Rivlin Material greatly expands the applicability of topology optimization. This study employs the open-source software Freefem++ to conduct displacement field analysis of nonlinear materials through the analytical sensitivity analysis. This is achieved by iterating through multiple iteration loops, ultimately obtaining the topological optimization results of Mooney–Rivlin and Neohookean Material by solving the respective adjoint problems.

Multi-scale, multi-rate damage and fracture: Models, experiments, and simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MULTISCALE CREEP MODEL CONSIDERING THE CONCURRENT EVOLUTION OF POINT DEFECT, DISLOCATION, GRAIN BOUNDARY, AND VOID

Yinan Cui[1] and Zhun Liang*[1]

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ABSTRACT

Creep poses a significant threat to the integrity and longevity of structural components at high-temperature. The most current understanding of creep mainly focuses on the coupled effect of point defects and dislocation, which may well describe the second stage of creep. However, the behavior of the three stages of creep is jointly contributed by point defect (vacancy) diffusion, dislocation glide, dislocation climb, GB sliding, and void evolution. A critical knowledge gap still exists regarding how these different creep mechanisms are simultaneously coupled during the different stages of creep. In this work, a multi-physical mechanism-based multiscale model is proposed to consider the concurrent evolution of point defect, dislocation, GB, and void based on a unified thermodynamic framework. In-situ scanning electron microscope (SEM) creep experiments and macroscopic creep experiments of Ti-6Al-4V were conducted to validate our model. The proposed model well predicts both the microscopic and macroscopic experimental creep behavior. The contribution of different microstructure evolution is discussed, and a phase diagram of the dominated creep mechanism is obtained This work not only deepens our understanding of the micro creep mechanism but also offers valuable insights for designing materials with specific microstructures to enhance their creep resistance.

Multi-scale, multi-rate damage and fracture: Models, experiments, and simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING BRITTLE MATERIALS WITH FLIP+MPM

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ABSTRACT

When brittle materials are involved in numerical simulations, the materials modeled will ultimately undergo fragmentation, that is, complete material failure and the opening of new physical crack surfaces. In order to simulate this phenomenal, a viscoelastic brittle material model (VBMM), an isotropic, orientation-independent model, is proposed to predict the initial stages of mechanical response, including material damage and viscoelasticity. However it will be challenging for Eulerian framework to simulate fragments due to failure. Therefore, by implementing this viscoelastic damage model into FLIP+MPM and applying simple failure criteria we can simulate processes where material catastrophically fails.

FLIP-MPM has significant advantages for solving problems that have large material deformations and has also been applied to many areas, such as material fracturing and fragmentation, fluid-structure interactions, and multiphase flows due to its multi-velocity capability.

In order to simulate the constitutive response of brittle materials, a viscoelastic strength and damage model were developed in the framework of Pagosa's FLIP+MPM. The model is calibrated over a variety of strain rates and calculates damage via growth of initial shear cracks to a critical size also taking tensile/spall criteria into account. The model also considers the nonisothermal condition. The temperature will change not only due to the inelastic work, but also the frictional heating (crack work). Here we will show the simulation by the viscoelastic brittle material model in FLIP+MPM/Pagosa and the (macro-damage) failure criteria.

Imaging-based methods in computational medicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NONRIGID IMAGE REGISTRATION OF LONGITUDINAL SUBJECT DATA TO QUANTIFY AGE-RELATED VENTRICULAR ENLARGEMENT

Lauren Cunniff[*1] and Johannes Weickenmeier*[1]

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ABSTRACT

One of the most prominent features of the aging brain is cerebral lateral ventricular enlargement caused by neurodegeneration-driven tissue volume loss. As such, ventricular changes are considered a valuable marker to distinguish between healthy aging and neurodegenerative diseases. Therefore, we developed a novel approach to extract lateral ventricular shape changes from longitudinal magnetic resonance images via nonrigid registration and quantify corresponding mechanical loading of the ventricular wall. Our registration approach utilizes rigid, affine, and nonlinear registration to obtain true ventricular deformations between two longitudinal images. Rigid registration facilitates broad global alignment, allowing subsequent affine and nonlinear registrations to capture age-related differences rather than positional disparities. We utilize FSL-based registration algorithms to provide the final deformation field between scans. To enable comparison between subjects, we created a template model of the ventricle based on segmentation of the MNI-152 brain atlas. We deform the template model to fit each subject’s baseline scan using our registration framework and subsequently map the subject’s displacement field onto the mesh. This allows us to compare ventricular deformations among subjects as well as to perform statistical analysis across our subject pool. In a final step, we compute area stretch and thickness changes of the ependymal cell layer forming the ventricular wall as measures of the mechanical loading of the ventricular wall.

We selected 50 healthy subjects from the Alzheimer's Disease Neuroimaging Initiative based on their age at baseline (70-75 years) and a follow up scan 4-5 years later. The ventricular deformations between the initial and follow-up scans revealed mostly uniform expansion during the observation period. Some local features include (i) pronounced wall strains along the ventricle’s edges of the main body and (ii) above-average curvature changes in the anterior and posterior horns. Strikingly, regions of higher mechanical loading coincide with locations commonly associated with periventricular white matter hyperintensities. This suggests that periventricular white matter hyperintensities are possibly caused by increased mechanical loading of the ventricular wall.

Architected materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TWO-SCALE DATA-DRIVEN DESIGN FOR HEAT MANIPULATION

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ABSTRACT

Data-driven methods have gained increasing attention in computational mechanics and design. This study investigates a two-scale data-driven design for thermal metamaterials with various functionalities. To address the complexity of multiscale design, the design variables are chosen as the components of the homogenized thermal conductivity matrix originating from the lower scale unit cells. Multiple macroscopic functionalities including thermal cloak, thermal concentrator, thermal rotator/inverter, and their combinations, are achieved using the developed approach. Sensitivity analysis is performed to determine the effect of each design variable on the desired functionalities, which is then incorporated into topology optimization. Geometric extraction demonstrates an excellent matching between the optimized homogenized conductivity and the extraction from the constructed database containing both architecture and property information. The designed heterostructures exhibit multiple thermal meta-functionalities that can be applied to a wide range of heat transfer fields from personal computers to aerospace engineering.

SPARSE BAYESIAN NEURAL NETWORKS FOR NONLINEAR TIME SERIES PREDICTION: TACKLING OVERFITTING AND UNCERTAINTY QUANTIFICATION

Nastaran Dabiran[*1], Brandon Robinson[1], Rimple Sandhu[2], Mohammad Khalil[3], Dominique Poirel[4] and Abhijit Sarkar[1]*

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ABSTRACT

Neural networks (NNs) demonstrate impressive expressivity to mimic the dynamics of complex systems, thereby offering a promising predictive model. In pursuit of enhanced predictive accuracy, there has been a trend toward increasing parameters in these networks, which has introduced significant challenges. A primary concern is overfitting, where the model becomes too tailored to the training data and fails to generalize well to unseen data. With the increase in parameters, the computational demand also rises.

While many approaches have been proposed to resolve this issue, they often fail to adequately address the complexity inherent in such models. This leads us to a critical question: how can we effectively choose the complexity of NNs while ensuring robustness and reliability in their predictions? To address this critical question, the focus shifts toward finding a balance between model complexity and data-fit. Leveraging insights from a hierarchical Bayesian setting in which the priors are conditional on hyperparameters, we construct a Bayesian NN (BNN) by applying a semi-analytical framework known as nonlinear sparse Bayesian learning [1]. This network aims to address the practical and computational issues associated with BNNs by imposing a sparsity-inducing prior that encourages the automatic pruning of redundant parameters based on the concept of automatic relevance determination (ARD).

This network is designed to leverage a hybrid prior [1], facilitating the use of a combination of ARD priors and informative priors. This configuration is advantageous for problems in computational mechanics as it permits the incorporation of relevant knowledge of the underlying system. Additionally, a Gaussian mixture model approximation of posterior distribution as a function of hyperparameters enables semi-analytical calculation of Bayesian entities. This reduces computational complexities typically associated with BNNs. The sparse BNN (SBNN) algorithm eliminates redundant parameters by optimally selecting the precision of the ARD priors, identifying the optimal sparse NN, effectively addressing overfitting. To demonstrate the benefits of the SBNN, we introduce an illustrative regression problem and contrast the results with a BNN using standard Bayesian inference and hierarchical Bayesian inference. Sparse Bayesian recurrent neural networks and Long Short-Term Memory will then be applied for the prediction of dynamical systems; a nonlinear oscillator inspired by the aeroelastic dynamics of airfoils in wind tunnel experiments, and compartmental model for COVID-19.

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Imaging-based methods in computational medicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICS-INFORMED MACHINE LEARNING AND MOLECULAR DYNAMICS OF COMPUTATIONAL DIFFUSION MAGNETIC RESONANCE IMAGING

Michael Dada[1], Bamidele Awojoyogbe*[1] and Nicholas Udeme*[1]

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ABSTRACT

In this talk, we present the viability of adding physics-based limitations into neural networks for image processing applications and the ability of Physics-informed neural networks (PINNs) to identify and extract relevant features from medical images, utilising the underlying physical properties of the imaging modality for more accurate feature representation, and evaluating the effectiveness of PINNs in reducing noise and artefact pre-selection.

There is no molecular situation where diffusion may be completely ruled out. The observed molecular dynamics are a product of all conceivable events occurring in the sample. Attempts to derive NMR diffusion from the Bloch NMR flow equations have been made [1]. The magnetic resonance signals detected from molecular dynamical processes derived in term of molecular diffusion is the focus of this presentation.

The goal is to develop physics-informed neural network algorithms for feature extraction, denoising, and segmentation of diffusion magnetic resonance signal (images) based on (i) physics-guided feature extractions (ii) strategies inside neural networks that rely on physics-based models to decrease data noise (iii) segmentation tasks, that include physical limitations in neural networks (iv) model performance in terms of peak signal-to-ratio (PSNR) and structure similarity index (SSIM).
These involve accurately defining boundaries or regions of interest, as well as performing comprehensive quantitative and qualitative studies to compare the performance of the PINNs method to traditional approaches and other deep learning techniques. Metrics including accuracy, sensitivity, specificity, and processing efficiency will be employed.

By incorporating the underlying physical laws driving the data, PINNs may increase segmentation accuracy, particularly in instances where conventional, exclusively data-driven algorithms may fail owing to noise or a lack of annotated data. Since medical imaging data are expensive or complicated, incorporation of physics-based constraints inside neural network topologies has the potential to reduce dependency on vast amounts of labelled training data which could be beneficial.
Combining physics principles with neural networks for feature extraction, denoising, and segmentation may pave the way to new insights and breakthroughs in fundamental medical imaging knowledge, showing relationships and patterns in medical data that would not be evident using traditional methodologies.

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AN INTEGRATED PHASE-FIELD LATTICE BOLTZMANN MODEL OF IMMISCIBLE TWO-PHASE FLOW AND HEAT TRANSFER AT THE TWO-PHASE INTERFACE WITH TEMPERATURE JUMP

Jialin Dai[12], Yumei Yong[1], Hanyang Mo[13], Wenqiang Chen[12], Menghui Li[4] and Chao Yang[1]*

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ABSTRACT

Abstract:
The temperature jump at the gas-liquid interface existing during the boiling and evaporation process reduces the internal heat transfer[1]. It is a changelling issue to accuratly capture both two-phase interface and the heat transfer at the two-phase interface because of the rapidly changing interface and different thermophysical properties of two phase. The developed phase-field lattice Bolzman method (pf-LBM)could simulate the immisble two-phase flow. Two energy equations for two phase coupling with pf-LBM is applied to the two-phase flow and heat transfer considering little interface that the computationl cost is high. We borrowed the idea of the concentration change method [2] for the mass transfer at two-phase interface and extended it to two-phase flow and heat transfer process. An energy equation was developed to express the heat transfer process for two phase and two-phase interface. Therefore, it can describe the temperature jump of interface, which is significant for non-equilibrium gas-liquid heat transfer. The new energy equation was integrated with pf-LBM. The integrated mathematical model was fully validated using a thermally stratified Poiseuille flow driven by external forces, thermal capillary flow in microchannels, and droplet migration driven by temperature gradients. The results were in good agreement with the analytical solution.

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Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DISCRETE ELEMENT SIMULATION OF POWDER SPREAD AND OPTIMIZATION

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ABSTRACT

Discrete element modelling (DEM) was used to simulate the process of spreading the Inconel718 powders. Firstly, based on experimental observations, we set up individual powder models with different sizes and shapes. Then powder test, including Pouring Heap, Hall Flowmeter, Revolutionary Powder Analyzer, were simulated to extracted the intrinsic properties, such as the friction coefficients and adhesion strengths. Afterwards, the powder spread process was simulated to deposit powders onto a working platform. In order to achieve high packing density, we characterized various conditional parameters, including blade sliding rate, shape effect, etc. Especially, we studied various blade geometries, such as inclined front surface, flexible cantilever beam, cylindrical roller. With carefully tuning parameters and characterizing packing density, we concluded that the optimized powder packing density was attributed to a combination of regular powder shape, slow sliding rate, and thin blade with slight inclined front surface. Our findings predicted an effective means of powder spreading process so as to serve as the benchmark of Additive Manufacturing technology.

Multiscale modeling, analysis and numerical methods of material defect and inhomogeneities
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NONLOCAL ELASITICITY MODEL FOR SIMULATING THE STRUCTURE AND STRESS OF CRYSTALLINE DEFECTS

Shuyang Dai[*1] and Xiaoyin Wang*[1]

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ABSTRACT

In this work, we present a nonlocal model in order to solve the static and dynamic problems related to crystalline defects such as dislocations, interfaces, etc. In our model, a superposition framework based on nonlocal description is used to solve the stress and displacement field due to defects. The interaction of dislocation with other types of defects such as cracks can be modeled with higher accuracy due to the consideration of nonlocal effects. The model is sovled by optimiaztion based numerical techniques in order to acclerate the simulations. We also apply this model to problems related to crystal interfaces.

Recent advances in meshfree and particle methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RESEARCH ON SPH MODEL FOR PREDICTING DEPOSITION EFFICIENCY OF COLD SPRAY

Zhen Dai[1], Fei Xu[1], Jiayi Wang[1] and Wei Feng[1]*

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ABSTRACT

Cold spray is a solid-state material deposition technique widely used in the repair and coating of metallic components, where understanding and optimizing the corresponding deposition efficiency of process parameters is crucial for process improvement and coating performance. The research commenced with the establishment of a GPU SPH model that simulates the high-velocity impact of particles during the cold spray process. This model incorporates the CS interface force that describes dynamic contact to predict the deposition efficiency based on the adhesive strength of the CS interface force. Results from the simulations showed a high correlation with the experimental data in the literature, demonstrating the model's robustness in predicting particle deformation and bonding conditions, which are essential for determining deposition efficiency. The effects of particle characteristics and process parameters on deposition outcomes were systematically analyzed, revealing that particle temperature and velocity are pivotal in achieving optimal deposition efficiency. The conclusions drawn from this study indicate that the SPH model is a viable tool for predicting deposition efficiency in cold spray processes. This predictive capacity not only provides a deeper understanding of the complex interactions during particle impact but also serves as a foundation for optimizing process parameters without extensive experimental testing.

Keywords: Cold spray, SPH model, deposition efficiency, CS interface force, process parameters.

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New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTATIONAL DESIGN OF 2D AND 3D NANOSTRUCTURES

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ABSTRACT

The advancement of nanotechnologies has been clearly driven by the discovery of novel nanomaterials and new nanofabrication routes. Research in nanostructured materials is an emerging field in which revolutionary devices can be designed with unique characteristics using nano-engineered structures as building blocks (Mitchell et al., 2020). This emerging field operates within the 1 to 100 nanometer scale, where morphology, shape, and structure determine material properties.

To successfully obtain nanostructures with tailored properties, different approaches need to be considered. Recently, a new topology-based machine learning method was proposed to predict materials' properties. Another approach, namely Nano-Topology Optimization, was presented to manipulate atom-by-atom to maximize elastic constants. Despite previous studies in designing optimized nanostructures, the use of TO methods at the nanoscale is still in its infancy.
This study proposes a formalized topology optimization method for nanomaterial design. Our approach combines molecular modeling using the LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) package (Plimpton, 1995) with the TOBS (Topology Optimization of Binary Structures; (Sivapuram & Picelli, 2018)) method to design nanostructures with unique mechanical properties.

Here, we present optimized metal nanostructures with unique mechanical properties obtained through a coupling of molecular modeling and the topology optimization method. Single and multiple objective functions were employed to design optimized 2D and 3D nanostructures. Our results demonstrate that their elastic properties can be easily tuned by coupling both approaches with proper constraints. Our results confirm that the coupling between molecular modeling and TOBS is promising for finding optimized designs with enhanced properties. This approach can be extended to more complex problems, including maximizing elastic constants with multiple objective functions and constraints and designing nanofluidic channels to minimize energy dissipation.

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Current trends in phase-field modeling and computations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NEURAL NETWORKS MEET PHASE-FIELD: A HYBRID FRACTURE MODEL

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ABSTRACT

For the mechanical behaviour of elastomers, micromechanically-informed constitutive models that are based on statistical mechanics have proven of high value, for instance the non-affine unit sphere model [1]. However, these approaches are computationally expensive. Likewise, for the prediction of fracture, the phase-field approach has become a well-established tool, although it comes along with a severe computational effort.

Physics-augmented neural networks (NNs) become increasingly popular for constitutive modelling, and have shown to be suitable surrogates for hyperelastic materials, see e.g. [2]. Apart from their flexibility for describing complex experimentally-observed material responses, these approaches may also reduce computational effort compared to classical micromechanically-informed models.

This contribution aims at combining the predictive capability of the phase-field approach to fracture with the advantages of NNs by means of a hybrid model of fracture. To this end, conceptionally similar to [3], a pseudo-energy functional is introduced, and as contributions to this functional, a neural network-based free energy potential and the classical phase-field fracture dissipation potential are considered.

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Advances in damage & fracture modeling of multiphysics materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MACHINE LEARNING-AIDED DIGITAL TWINS FOR DAMAGE SENSING: A MULTI-PHYSICS AND MULTI-SCALE COMPUTATIONAL FRAMEWORK USING PIEZOELECTRIC COMPOSITES

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ABSTRACT

Failure of composite materials is inherently a multiscale phenomenon. It is governed by damage mechanisms at the microstructural length scale of the material. These damage mechanisms determine the initiation and evolution of fracture across length scales, manifesting its effects on the structural response. This necessitates the development of a robust sensor that can quantify the characteristics of material damage. Piezoelectric composites are an obvious choice for this application due to a strong electromechanical coupling. This work attempts to advance our understanding of damage and develop a tool to predict it. A micromechanical model for crack evolution in heterogeneous piezoelectric composite microstructures is developed. Crack propagation and interfacial decohesion in the presence of electro-mechanical fields are modeled by a phase-field model integrated with cohesive traction-separation laws at material interfaces. However, high gradients in the solution fields require a fine discretization of the computational domain leading to increased computational cost. The first part of the work implements an adaptive wavelet-enhanced hierarchical framework to improve the efficiency of the finite element solver. Numerical examples are solved to demonstrate the advantage of this technique over conventional methods.

Simulating damage in structural scale components using a high-fidelity phase field model is computationally intractable. Therefore, a generalized higher-scale continuum damage mechanics model for piezo-composite structures is introduced in the second part of the work. Evolution laws are formulated to model damage growth at the component scale with evolving mechanical and electrical fields. A nonlocal scheme is included in the finite element implementation to alleviate mesh dependency in the simulations. Numerical examples are solved to demonstrate the macroscopic effects of damage on the structural response.

The strong electromechanical coupling in piezoelectric materials leads to the third part of the work which develops the digital twin of a damage sensor. This can quantitatively predict microstructural damage from the measurement of macroscopic electrical signals at predefined locations on the surface of the structure. An advanced machine learning model capable of treating history-dependent nonlocal material data is employed for this purpose. This model can replace current practices of damage sensing techniques by providing a quantitative global damage indicator in near-real time rather than a location-specific qualitative damage measure.

Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CONTINUOUS-DISCONTINUOUS ANALYSIS OF FATIGUE FAILURE USING THE DISCONTINUITY STRAIN METHOD

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ABSTRACT

Fatigue failure analysis involving crack initiation and propagation is numerically challenging as the pre-crack mechanism is governed by continuum mechanics, while the post-failure behavior falls into the category of contact mechanics. Although either continuous or discontinuous models are frequently employed to describe the process, none of them is adequate when considered alone. Discontinuous models use strong discontinuities to resemble sharp cracks, yet they are not well equipped to describe diffuse damage arising from micro-crack nucleation. Ductile damage models, on the other hand, render the deformation of the failed region to be irreversible, leading to unphysical behavior upon unloading. The reason lies in the fact that continuum straining continues after complete failure, which gives rise to the accumulation of plastic strain across the failed region. Thus, neither stress redistribution nor the unloading branch of global responses can be correctly captured. We provide a solution for those issues by augmenting the conventional additive strain decomposition of the infinitesimal strain theory. We introduced a discontinuity strain to the conventional elastic-plastic strain decomposition to absorb the unphysical continuum strains across the failed region [1, 2]. Accordingly, no further plastic straining occurs, leading to more realistic local and global responses. This augmentation neither invokes a major modification of the constitutive model nor increases the computational efforts associated with crack closing and reopening effects. Although the method can be employed in conjunction with any kind of material model, we use simple ductile damage to introduce the idea. We adhere to this strategy to keep the complexity arising from constitutive modeling minimal. After presenting the theoretical and algorithmic aspects of the method, it is validated against established experimental benchmarks from the literature, showing its robustness in fatigue failure analysis and potentially in other phenomena invoking the representation of discontinuities along with ductile damage formulations.

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Advanced materials: Computational analysis of properties and performance
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPLORING PLASTIC DEFORMATION BEHAVIOR IN NANOTWINNED METALS UNDER HIGH QUASI-HYDROSTATIC PRESSURE: A MOLECULAR DYNAMICS INSIGHT

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ABSTRACT

Conventional plasticity theories have long held that hydrostatic pressure merely results in volumetric changes in solids without inducing plastic deformation. However, our studies here reveal a fascinating deviation from this conventional understanding as exemplified by nanotwinned (NT) metals. Using X-ray diffraction (XRD) and transmission electron microscopy (TEM) techniques, we have found detwinning phenomena in Cu-10wt.%Ni NT metals under high quasi-hydrostatic environment (~11.5GPa) applied by using diamond anvil cells. In addition, there exist a significant grain growth and a reduction in the number of twins, which are key indicators for plastic deformation behavior of the NT material under hydrostatic pressure. To comprehensively understand these phenomena, we have conducted large-scale molecular dynamics (MD) simulations to explore the plastic deformation behavior of NT metals under such extreme loading conditions. Remarkably, our MD simulations unveil a compelling insight: the presence of grain boundaries and twin boundaries leads to localized stress concentrations, ultimately resulting in plastic deformation at the nanoscale. Such behavior is quite unconventional according to the conventional plasticity theories under hydrostatic pressure. These results not only corroborate our experimental observations and but also expand our understanding of material behavior under extreme conditions. Furthermore, the present study not only sheds light on the unique plastic deformation mechanisms in NT metals but also challenges the conventional plasticity theories, advocating for the expansion of their boundaries , which may open up new directions for material design and engineering.

Computational modeling of extreme-loading events
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PERFORMANCE OF ARBITRARY-ORDER FINITE ELEMENTS IN NONLINEAR LUMPED-MASS EXPLICIT DYNAMIC ANALYSIS

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ABSTRACT

For over a decade, higher-order finite elements have proven to be effective for lumped-mass explicit methods in highly nonlinear solid dynamics, including contact/impact applications, and have increasingly become available in popular codes [1-3]. These elements have distinct advantages that can naturally represent curved shapes, model flexure without significant shear locking or artificial spurious hourglass control/special modes (e.g., incompatible, assumed strains, etc.), and can facilitate locking treatments for nearly incompressible materials. Nevertheless, use of lumped-mass higher-order elements generally is still far less than that of the traditional first-order ones. This is especially the case with increasing orders, as the LS-DYNA and IMPETUS AFEA codes have only first-, second-, and third-order solid elements. Hierarchical finite elements can provide improved performances using higher-order enriched basis functions but are not amenable to mass lumping. Similarly, more recent IsoGeometric Analysis (IGA) can exhibit tremendous smoothness benefits but also loses some of its effectiveness in lumped-mass explicit methods. This area is continuing to mature, but smoothness and lumping seem to be opposing mechanisms. Classical Lagrange elements, however, can effectively strike a balance by permitting C0 discontinuity, important in many typical high-rate explicit applications like fragmentation and penetration, while also providing element curvature and increased smoothness via higher-order polynomials. Whereas an effective diagonal lumped-mass central difference time integration is still used, the critical time increment can decrease non-proportionately with increased element order, particularly due to increasingly closer inter-nodal locations used to improve basis accuracy. In this presentation, an examination of the performances of arbitrary-order finite elements in lumped-mass explicit methods is made particularly with regards to basis order and nodal placement. This study uses both single element and other simple analyses as well as common benchmark and practical high-rate applications using various elastic, hyperelastic, and elastic-plastic material models.

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Modeling and simulation of advanced manufacturing processes for metals
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFECT OF INTERPASS TEMPERATURE ON RESIDUAL STRESS EVOLUTION IN A NICKEL-ALUMINUM BRONZE WIRE-ARC ADDITIVE MANUFACTURING BUILD

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ABSTRACT

Nickel-aluminum bronze (NAB) alloys are commonly used for marine applications such as propellers and valves. Recent interest has shifted to replacing conventionally cast NAB components with those fabricated using large-scale, wire-arc additive manufacturing (WAAM) processes. However, residual stresses and part-level distortion in as-built parts can contribute to build failures and reduced performance in components produced by additive manufacturing (AM) techniques, which hinders process qualification and part certification due to reduced performance. Implementation of higher interpass temperatures are being investigated as a mitigating technique to reduce distortion and residual stresses. This study used commercial AM simulation tools to analyze how differing interpass temperatures can influence the as-built residual stresses in a WAAM-built NAB part. The predicted results were validated using the contour method to quantify the amount of residual stress in the selected component.

Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OF CELLULAR STRUCTURES WITH THE TARGETED NON-LINEAR MECHANICAL RESPONSE

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ABSTRACT

With the advent of advanced additive manufacturing capabilities, it is feasible to create sophisticated cellular structures using diverse materials such as polymers, metals, and ceramics. By altering the topology of the unit cell, a mechanical property can be modulated without changing the material composition. Nevertheless, identifying an optimized topology within an enormous design space that would precisely deliver the targeted non-linear material response is challenging. We have developed a data-driven machine-learning approach capable of reverse-engineering the topology of a cellular structure based on the intended material response in linear as well as non-linear regimes. Our method involves two steps: (a) generating new topology using cellular automata, enabling a database of cellular structures for assessing the structure-property relationship, and (b) reverse-engineering the unit cell topology from the desired non-linear stress-strain data using a generative machine learning framework. This work has potential applications in identifying novel structures with mechanical specifications requiring complex materials response suitable for applications requiring optimized energy absorption, damping attenuation, and impact mitigation.

Advances in damage & fracture modeling of multiphysics materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTI-PHASE-FIELD MODELLING FOR AM PROCESSES SIMULATION INCLUDING IN-SITU THERMAL FRACTURING

Roya Darabi[1], Ana Reis[1] and Jose Cesar de Sa[1]*

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ABSTRACT

In the realm of engineering, tackling the intricate challenges associated with thermal fractures in metal additive manufacturing stands as a formidable task. This study harnesses the capabilities of parallel modeling and the Multi-App feature within MOOSE, presenting a comprehensive solution to this multifaceted issue.

Our methodology involves the seamless coordination of both the Main-App and sub-applications to delve into the intricacies of thermal fracture modeling. The Main-App focuses on simulating the underlying physics, encompassing processes such as heating, phase change from powder to liquid state, and solidification. This is achieved through the application of the Allen-Cahn phase field, coupled with an elastoplastic model, all facilitated by the Multi-physics Object-Oriented Simulation Environment (MOOSE). Following this, the data seamlessly transitions to the sub-application for a meticulous analysis of thermal fractures. Specifically tailored to model liquation cracks in Martensitic alloys, the sub-application utilizes diffusive phase field crack modeling, incorporating an additional energy scale of Allen-Cahn to control non-conserved damage evolution.

Efficiency and computational time optimization are realized through the implementation of a staggered method for process synchronization, ensuring the smooth exchange of data between the Main-App and sub-application. Additionally, an adaptive mesh is employed to finely control the interface, guaranteeing precise and accurate modeling of thermal fracture dynamics.

The findings of this study illuminate the impact of process parameters in additive manufacturing and their inherently complex multiscale nature. The ultimate aim is to identify optimal conditions and minimize imperfections in the pursuit of enhancing the overall efficiency and quality of metal additive manufacturing processes.

Coupled computational mechanics: Solutions for FSI simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A PROJECTION-BASED FILTERING STRATEGY FOR QUASI-NEWTON INTERFACE METHODS IN FLUID-STRUCTURE INTERACTION

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ABSTRACT

Problems involving multiphysical interactions, such as fluid-structure interaction (FSI) require the imposition of interface coupling conditions between the component systems. The extent of interface coupling to be enforced is dependent on the potential instabilities arising as a consequence of the interactions between the systems. A partitioned approach allows for maintaining flexibility and modularity with regard to solving the individual physical systems independently while compromising on the extent of coupling between the systems. In this regard, the coupling is achieved through the formulation of a fixed-point problem. Relaxation strategies have been observed to be slow to converge. The interface Quasi-Newton method (IQN-ILS) [1] based on Anderson mixing has succeeded in accelerating convergence of the fixed point problem involving elastically deforming structures at moderate mass ratios. However, in FSI systems involving low-mass ratios, the problem of coupling the fluid-structure systems is accentuated by the added mass instability [2], and demands an efficient convergence acceleration strategy. The proposed non-linear iterative force correction method illustrated excellent performance in the case of elastically mounted structures with low mass ratios.

The IQN-ILS method involves the formation of an inverse Jacobian whose quality is detrimental to the performance of the method. In this regard, it is essential to ensure linear independence of the residual vectors constituting the secant pairs used in the method. In the current work, we present a method of filtering based on the approximate inverse Jacobian which eliminates redundant data from previous iterates. Simultaneously, we construct a projection-based strategy which regulates no redundant data enters into the computation of inverse Jacobian. Furthermore, this ensures the Anderson acceleration method always attempts to update the solution along new vectors at every iteration. We demonstrate the reduced iteration count, and lower cost [3] involved in the Turek-Hron FSI benchmark for a range of mass ratios.

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Phase-field modeling: Analytics, benchmarks, and discussions
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ON A COUPLING TECHNIQUE BETWEEN CALPHAD DATABASES AND A GRAND-POTENTIAL-BASED PHASE-FIELD MODEL: THEORY AND APPLICATIONS

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ABSTRACT

In phase-field simulations of phase transformation reactions in material systems, an accurate obtaining of relevant thermodynamic properties has been a matter of interest. Slight deviations in these properties can lead to enormous discrepancies in the finally evolved microstructures. The Gibbs free energies are among the main factors in this context. To achieve Gibbs free energy functions, Calphad thermodynamic databases are widely used which are constructed based on the applicable theoretical and experimental information on phase equilibria for the specific systems. Different coupling approaches are introduced between these databases and the phase-field models in the literature. The direct implementation of the Gibbs energy functions in the simulation model can exemplarily be mentioned. As an alternative method, the necessary thermodynamic data can be achieved from the databases instantly. In the present investigation, it is shown that such methods are not deemed suitable within the framework of the considered grand-potential-based phase-field model. To reduce the computational effort in solving the higher order mathematical expressions of the Gibbs energy formulations, a workflow is presented to approximate the Gibbs energy expressions in the form of second-order polynomials depending on the temperature and composition. It is shown that these functions can represent the Gibbs values and the chemical potentials quite accurately in a range close to thermodynamic equilibriums. As practical utilizations of the introduced method, the eutectic reactions in different binary and ternary material systems are simulated. Eutectic solidification in NiMo, NiAlMo, and BiInSn systems are discussed under Directional and/or Rotating Directional Solidification (DS-RDS) conditions. As an important parameter study, the effects of anisotropic interfacial properties on the formed patterns are studied and convincing correlations with the experimental and theoretical anticipations are achieved. Self-propagating High-temperature Synthesis (SHS) is another process that is investigated in NiAl and RuAl systems. The evolving polycrystalline grain microstructures reveal convincing agreements with the available experimental data. Altogether, the achieved results demonstrate the applicability of the established coupling method between the Calphad databases and Grand-potential-based phase-field approaches.

Numerical methods, mathematical modeling and analysis in material science
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LARGE-SCALE MATERIALS MODELLING USING DFT-FE

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ABSTRACT

Large-scale Kohn-Sham density functional theory (DFT) calculations involving tens of thousands of electrons are critical required in variety of application areas, which include extended defects in metals and semiconductors, low-symmetry layered materials, large-scale bio-molecular simulations, and many others. However, the stringent accuracy requirements in DFT needed to compute meaningful material properties, in conjunction with the asymptotic cubic-scaling computational complexity with number of electrons, demand huge computational resources. Thus, these calculations are routinely limited to material systems with at most few thousands of electrons. In this talk, I will present a massively parallel real-space DFT framework (DFT-FE) [1-3], which is based on a local real-space variational formulation of the Kohn-Sham DFT energy functional discretized with higher-order adaptive spectral finite-elements, and handles pseudopotential and all-electron calculations in the same framework. I will present the efficient and scalable numerical algorithms in conjunction with HPC centric implementation strategies for the solution of Kohn-Sham equations, that has enabled computationally efficient, fast and accurate DFT calculations on generic material systems reaching ~200,000 electrons. DFT-FE demonstrates an order of magnitude performance advantage over widely used plane-wave codes both in CPU-times and wall-times. Finally, I will discuss a successful large-scale application of DFT-FE to modeling of dislocations in crystalline materials, where we computed the core-energetics of pyramidal dislocations in magnesium and dislocation-solute interaction energies in presence of dilute Yttrium solute alloying. These core energetics are critical inputs to phenomenological modelling of ductility in magnesium alloys, but have so far been out of reach using plane-wave DFT codes. I will present accurate cell-size converged computation of these first-principles inputs that required simulation sizes reaching 3000-6,000 atoms (30,000-60,000 electrons), and has provided crucial insights towards predictive modelling of ductility in magnesium.

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Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

REGULARISED CONTINUUM DAMAGE MODELS

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ABSTRACT

Continuum damage models, typically those with an order parameter, are extremely useful in characterizing both 2D and 3D fracture in materials. They eliminate the necessity of ad-hoc criteria for fracture propagation and regularize a discontinuous crack by the use of a physically meaningful lengthscale. In this talk, there will be a discussion on the application of such regularized models to two problems. The first problem is that of pure brittle damage of elastomers. To solve this problem, we use a geometrically inspired approach where the kinematic quantities appearing in the strain energy takes into consideration the damage of the undeformed configuration. The resistive energy is a function of the Riemannian curvature that ensues from the assumption that the manifold is no longer Euclidean after damage commences. Through this approach, we are able to resolve numerically, a rapidly evolving singularity which is a challenge with all commonly available damage models. The second problem is that of a dynamic crack propagation through a 3D solid containing a tougher asperity. In this problem, the encounter with the asperity gives rise to solitonic crack front waves that travel unabated along the crack front. Contrary to earlier approaches that involved linear perturbation based analytical solutions or the cohesive zone approach, we are able to obtain a nonlinear object with both in-plane and out-of-plane components. The fact that a front wave comprises of both in-plane and out-of-plane components is consistent with experiments and analysis of post-mortem fracture surfaces. Complexities in both these problems are manifold, yet the regularized models are able to resolve them elegantly, with reasonable numerical effort.

Numerical modelling of composite materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SIMPLIFIED CONSTITUTIVE TENSOR MODEL FOR THIN-WALLED FERROCEMENT WALL SYSTEM SIMULATION

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ABSTRACT

The thin-walled ferrocement wall system has been shown to provide earthquake-resistant properties usable in housing structures through experimental tests. Experimental tests, applied to walls built on a full scale, allow structural parameters to be identified and the capacity and performance of walls under static load to be evaluated.
Previously, constitutive models have been proposed based on an isotropic damage model for modeling the mortar and the classical elasto-plasticity theory for modeling the reinforcing bars and mesh. The combination of the models, through mixing theory, allows reflection of their mechanical behavior for implementation in numerical simulation. The models' complexity and interaction lend itself to using code developed expressly for this type of simulation restricting their use to research purpose.
This document establishes a methodology for simulating thin-walled ferrocement walls through commercial programs using a simplified model for their characterization and analysis, whose input will be the constitutive matrix of the composite material assigned to each finite element. The constitutive matrix of the composite material will be computed considering the percentages of volumetric participation of the simple materials that compose it and the working orientation of the fiber-type materials through the serial/parallel mixing theory.

Keywords: Ferrocement Walls, Series/Parallel Mixing Theory, Numerical Simulation

Enabling technologies for digital twins: Model reduction and scientific machine learning
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PROJECTION-BASED MODEL ORDER REDUCTION OF ENVIRONMENTAL FLOWS USING FEM-BASED VARIATIONAL MULTISCALE METHOD

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ABSTRACT

The simulation of environmental flows presents a formidable challenge due to the inherent complexity of natural phenomena and the high computational cost associated with traditional modeling approaches. In this study, we propose a framework for the efficient and accurate simulation of environmental flows through projection-based reduced order models (ROMs) within the framework of finite-element method (FEM) and variational multiscale (VMS) modeling [1]. The POD-Galerkin approach is used to construct ROMs that capture the dominant flow features while significantly reducing the dimensionality of the problem. By extracting the most informative modes from high-dimensional flow data, the POD-Galerkin ROMs provide a compact representation of the flow dynamics, enabling faster computations while retaining essential physical insights. To assess the efficacy of our approach, we validate the projection-based ROM framework on standard benchmark cases such as lid-driven cavity, vortex shedding behind a 2D cylinder and turbulence generation on a 2D backward-facing step. Additionally, we demonstrate the applicability of the proposed methodology to real-world environmental flow problems, showcasing its versatility and utility in addressing complex flow dynamics scenarios encountered in environmental sciences and engineering. Through rigorous validation and application to diverse flow scenarios, we demonstrate the effectiveness and potential impact of the proposed approach in facilitating computationally affordable yet accurate simulations of environmental flows.

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SIMULATION OF PARTICLE-LADEN FLOW ON AN INCLINED PLANE WITH VARYING TOPOGRAPHY

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[1]*University of California, Los Angeles*

ABSTRACT

We develop a dynamic model to investigate mixtures of particles and viscous fluid on an inclined plane with varying topography. Our model accounts for several important factors, including gravity-induced settling of particles, particle resuspension due to shear-induced migration, the liquid surface tension, and the topography profile. In the thin film limit, we derive a reduced model consisting of hyperbolic-type equations for the liquid layer thickness and particle volume fraction. The resulting equation depends only on the direction parallel to the inclined plane, making it easier to solve compared to the governing equation while still capturing its essential features. A noteworthy aspect of our study is the incorporation of additional terms in the reduced model, which consider the influence of the normal component of gravity, surface tension, and variations in the topography. This inclusion allows us to gain a deeper understanding of how these factors influence the dynamics of the system. We analyze several cases of topographical variations, such as sinusoids, Gaussians, and sharp steps, using both theoretical and numerical approaches. These analyses hold significant practical applications, including the study of mudslides, microchip manufacturing, and material processing.

Trustworthy multi-fidelity and data-driven models for computational applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SURROGATE MODELING WITH DEEP RANDOM FOURIER FEATURES RESIDUAL NETWORKS AND MULTIFIDELITY INFORMATION

Owen Davis[1], Gianluca Geraci[2] and Mohammad Motamed[3]*

[1]*Sandia National Laboratories, University of New Mexico*
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[3]*University of New Mexico*

ABSTRACT

In this work, we consider neural network based surrogate construction leveraging multifidelity data. This is an active area of research that has promising applications in uncertainty quantification for high dimensional problems where conventional surrogate construction is computationally prohibitive. While this body of literature has grown markedly in recent years, there remain important deficiencies, two of which we address here. First, many of the current modeling paradigms are designed with bifidelity information in mind, and they do not present clear principled extensions in cases where we have an ensemble of lower fidelity information sources of know hierarchy in terms of their predictive capability of the true quantity of interest. Second, neural network based modeling paradigms rarely come with embedded and/or scalable uncertainty quantification procedures, which severely limits their utility in practical applications.

To address these shortcomings, we propose a multifidelity modeling paradigm capable of leveraging a hierarchical ensemble of lower fidelity information sources and with embedded uncertainty quantification. This paradigm is based on deep random Fourier features residual networks, which have similar approximation capability to ReLU networks[1], and makes fundamental improvements over our previously proposed bifidelity modeling paradigm based on one layer random Fourier features network[2]. In particular, the new method leverages a novel layer-by-layer global-optimization-free neural network training algorithm with error control. This algorithm utilizes and extends an adaptive Markov Chain Monte Carlo (MCMC) method developed for random Fourier features regression[3], and we leverage this MCMC based training to obtain computationally efficient uncertainty estimates updated after each layer of network training. We will illustrate our method's ability to leverage an ensemble of hierarchical lower fidelity information sources on an array of benchmark problems from the literature, and we will demonstrate the quality of our method's embedded uncertainty estimates on a surrogate modeling task related to quantum gate implementation for noisy intermediate scale quantum (NISQ) devices.

[1] O. Davis, G. Geraci, and M. Motamed. “Approximation error and complexity bounds for ReLU networks on
low regular function spaces”. In: (2024). Submitted.
[2] O. Davis, G. Geraci, and M. Motamed. “Multi-Fidelity Surrogate Modeling with Fourier Features Networks”. In:
Computer Science Research Institute Summer Proceedings 2023, S.K. Seritan and B.W. Reuter, eds., Technical
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(2020).

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UQ-TTA student paper competition in uncertainty quantification
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SURROGATE MODELING WITH DEEP RANDOM FOURIER FEATURES RESIDUAL NETWORKS AND MULTIFIDELITY INFORMATION

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To address these shortcomings, we propose a multifidelity modeling paradigm capable of leveraging a hierarchical ensemble of lower fidelity information sources and with embedded uncertainty quantification. This paradigm is based on deep random Fourier features residual networks, which have similar approximation capability to ReLU networks[1], and makes fundamental improvements over our previously proposed bifidelity modeling paradigm based on one layer random Fourier features network[2]. In particular, the new method leverages a novel layer-by-layer global-optimization-free neural network training algorithm with error control. This algorithm utilizes and extends an adaptive Markov Chain Monte Carlo (MCMC) method developed for random Fourier features regression[3], and we leverage this MCMC based training to obtain computationally efficient uncertainty estimates updated after each layer of network training. We will illustrate our method's ability to leverage an ensemble of hierarchical lower fidelity information sources on an array of benchmark problems from the literature, and we will demonstrate the quality of our method's embedded uncertainty estimates on a surrogate modeling task related to quantum gate implementation for noisy intermediate scale quantum (NISQ) devices.

[1] O. Davis, G. Geraci, and M. Motamed. “Approximation error and complexity bounds for ReLU networks on
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Report SAND2023-13916R, Sandia National Laboratories, 2023, pp. 278–293. (2023).
[3] A. Kammonen et al. “Adaptive random Fourier features with Metropolis sampling”. In: arXiv preprint arXiv:2007.10683

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16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics

July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

QUANTUM COMPUTING FOR FINITE ELEMENT PROBLEMS

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[2]*Florida State University*
[3]*Florida A&M University*

ABSTRACT

Quantum computing holds significant promise for revolutionizing computational approaches in various fields, including engineering and science. Its potential to solve finite element problems, which are computationally intensive on classical computers, stems from its ability to perform calculations at exponentially faster rates. This makes quantum computing particularly suitable for tackling large-scale and complex finite element analyses that are currently challenging or impractical with traditional methods.

In this talk, we will introduce solution algorithms for the two primary types of quantum computing architectures: quantum annealers and gate-based quantum computers. Quantum annealers are specialized for solving optimization problems. However, their application is limited to specific types of problems, and they require a large number of qubits for complex tasks. On the other hand, gate-based quantum computers are more versatile and capable of executing a wide range of algorithms. They promise exponential speedups for a broader set of problems, including those involving linear systems and differential equations. Despite these advantages, gate-based systems are currently more challenging to scale and require sophisticated error correction techniques. As these challenges are addressed, quantum computing is expected to unlock new possibilities in solving finite element problems with unprecedented efficiency and precision.

Recent advances in high-order methods for computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HIGH-ORDER, STRUCTURE-PRESERVING SCHEMES FOR MAGNETOHYDRODYNAMICS ON GPU ARCHITECTURES

*Joseph Dean**[1] *and Garth Wells*[1]

[1]*University of Cambridge*

ABSTRACT

Established codes for magnetohydrodynamics problems often rely on traditional, low-order discretisations of the Navier–Stokes equations and Maxwell's equations. These low-order methods have low arithmetic intensity, which is not well-suited to current and future generations of high-performance computing architectures. Simulation of complex, whole-system problems will require accurate and stable methods with high arithmetic intensity, especially to exploit the coming generation of exascale computers.

We investigate the application of high-order, structure-preserving methods for the magnetohydrodynamics equations on GPU architectures. These discretisations are stable, arbitrarily high-order accurate, conserve mass exactly, and yield exactly solenoidal magnetic fields, but present some challenges on GPU architectures due to the reliance on high-order H(div)- and H(curl)-conforming finite elements. High-order geometry is also required, which can result in both mathematical and computational difficulties. As an example application, we focus on liquid metal breeder blankets, which are used in some nuclear fusion reactor designs, and present results that examine the fraction of peak hardware performance that can be achieved. The solver makes use of recent developments in the FEniCSx finite element library.

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ACCELERATING CFD SIMULATIONS WITH ARTIFICIAL INTELLIGENCE (AI) – A PRACTICAL APPROACH

Manas Kumar Deb[*1] and Marcin Rojek*[2]

[1]*Capgemini*
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ABSTRACT

Throughout the past decade, we have been witnessing a strong and steady rise in the interest in applications of Artificial Intelligence (AI) and the associated Machine Learning (ML) techniques to help solve diverse scientific and industrial problems. One such area is computational mechanics where the focus has been to improve the time and cost efficiencies of complex, nonlinear, and multi-scale systems with the help of AI.

In general, Computation Fluid Dynamics (CFD) simulations involve nonlinear equations which require the use of numerical solvers and fine-scale domain discretization. This leads to high computational costs and long waiting times for results for such simulations. This burden is exacerbated even further in design optimization exercises where typically many simulations need to be conducted to find the optimal flow domain shapes and flow parameters/variables. These challenges make CFD a good target for investigation of potential use of AI.

As an active area of research there are now many publications on the topic of “AI in CFD” (see, for example, presentations from Steve Brunton [1] or Michael Bauerheim [2], and the references therein for a quick summary of problem formulation, solution techniques, and their pros and cons). As such, there are two high-level approaches through which AI can be applied to CFD simulation. The first, creating an alternate/surrogate CFD solver using AI that solves a problem equivalent to the original one, and the second, creating an AI-based layer alongside or surrounding the standard CFD solvers to accelerate the speed of the overall simulation, for example, by requiring fewer iterations or gaining faster convergence rates in an iteration.

The current presentation will focus on the use of AI to accelerate CFD simulations. We will present the overall construct of a self-optimizing AI layer which works in tandem with traditional CFD solvers (see [3] for some background information) making this approach easily adaptable to a wide variety of problems and without requiring a deep knowledge of AI/ML techniques. We will report details of the high (10x-40x) performance gains with this approach in benchmarked problems. We will also discuss the impact of the underlaying HPC hardware on the time/cost of the simulation.

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MODEL ORDER REDUCTION TECHNIQUES FOR THE PREDICTION OF VIBRATION IN THE BUILT ENVIRONMENT

Amar Pashov[1], Stijn Francois[1] and Geert Degrande[*1]*

[1]KU Leuven

ABSTRACT

Considerable progress has been made regarding the development of numerical models for the prediction of railway induced vibration, including 2.5D and periodic coupled FE-BE or FE-PML models of the track and soil, as well as 3D FE-BE models for buildings accounting for dynamic soil-structure interaction. These models are used to design vibration mitigation measures and to perform environmental impact studies.

Industry experiences a strong need to conduct extended parametric studies, to optimize vibration mitigation measures in a robust manner, and to perform forward stochastic predictions. These applications require prediction models that are fast to run. We therefore investigate the potential of model order reduction techniques such as Proper Generalized Decomposition [1] to tackle the curse of dimensionality.

The PGD formulation is based on the assumption of a separable form of the multi-dimensional field. Each contribution therefore consists of a rank-one tensor and is computed in a greedy manner. To this end, the PGD formalism is introduced into the weak form and the resulting non-linear problem is solved using fixed-point iterations. Damping terms result in non-Hermitian properties of the operator, hindering convergence of the standard Galerkin PGD approach. Therefore, alternative solution strategies, like Petrov-Galerkin based solvers, are considered [2]. We compare the classical greedy rank-one update with a greedy Tucker approximation method [3].

We elaborate the PGD formulation for three problems with different complexity: (P1) a simplified source model of a beam on Winkler foundation; (P2) a 2.5D model of a ballasted track on a heterogenous soil medium, modelled with finite elements in combination with complex frequency-shifted perfectly matched layers; (P3) Green’s functions for in-plane (P-SV) and out-of-plane (SH) wave propagation in a layered halfspace. Apart from the frequency and wavenumber, we take along the foundation stiffness (P1), ballast and soil properties (P2), or source and receiver positions (P3) as coordinates in the PGD formulation. The considered algorithms are compared in terms of convergence, memory requirements, and CPU time.

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Multi-scale modeling and upscaling for flow induced vibrations, from local reference simulations to certified industrial tools
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT OF A METHODOLOGY TO QUANTIFY THE DISTRIBUTION OF VIBRATION FREQUENCY AND DAMPING FOR SUBMERGED ELASTIC STRUCTURES

Joris Degroote[*1] and Henri Dolfen*[1]

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ABSTRACT

It is well-known that the free vibration frequency and damping ratio of elastic structures, like tube bundles or pump rotor blades, can be significantly different when submerged compared to in vacuum, due to the added mass and damping by the fluid. The complexity of the fluid mechanics in play makes purely analytical derivation of these effects difficult, so a numerical methodology has been established to quantify the submerged vibration characteristics in a reasonable time.

This methodology begins with the development of a time-dependent fluid-structure interaction model by coupling a finite volume flow solver to a finite element structural solver using a quasi-Newton coupling algorithm. The turbulence is modelled with an unsteady Reynolds-averaged approach, as a compromise between computational cost and fidelity. In this model, the structure is then deformed according to one of its eigenmodes in vacuum as initial condition. The free vibration resulting from the release of the structure is subsequently calculated, from which the modified vibration frequency and damping ratio can be extracted [1].

It can occur that the geometrical or operational parameters are uncertain, rendering the vibration characteristics uncertain too. To quantify this uncertainty, the approach mentioned above has been combined with polynomial chaos expansion [2]. This approach requires a number of repetitions of the simulation mentioned above, but the computational cost is reasonable for a handful of parameters, yielding a feasible approach to quantify the distribution of vibration frequency and damping. This new methodology has been validated for the first mode of a flexible tube with uncertain bow in a bundle.

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Physics-informed machine learning for numerical modelling in engineering and science
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADAPTIVE WEIGHT TUNING OF PHYSICS-INFORMED NEURAL NETWORKS WITH HARD BOUNDARY CONDITION IMPOSITION FOR FAST AND ACCURATE INVERSE ANALYSIS

Shota Deguchi[*1] and Mitsuteru Asai*[1]

[1]*Kyushu University*

ABSTRACT

Data-driven approaches have found widespread applications in various domains, including the field of computational engineering. In recent years, the use and development of machine learning methods have attracted much attention.
While many machine learning models learn only from a large amount of observed data, the recent trend involves the active development of models to exploit well-established expert knowledge. For physics problems, many models have been proposed to integrate limited data and physical laws, with physics-informed neural networks (PINN) [1] attracting particular attention. PINN integrates known physical laws modeled by the governing equations, making it applicable to both forward and inverse analyses, which is particularly advantageous when the available data is scarce.
In the original formulation of PINN, the loss function is composed of several terms: the difference from observed data (observation loss), the error in fitting the boundary condition (boundary condition loss), and the residual of the governing equations (physics loss). In this formulation, the boundary condition is considered only in a “soft manner”, by adding a penalty term to represent the boundary condition error. The accuracy of PINN solutions is strongly dependent on the penalty coefficient, and therefore, it is effective to impose the boundary condition in a “hard manner” [2]. However, when applied to inverse analysis, penalty terms are still needed to define the observation that is sensitive to the penalty coefficient, although it is difficult to estimate the appropriate range before training. To address this, an adaptive weight tuning method [3] has been shown to be effective.
In this study, with a special focus on inverse analysis, we present a hybrid technique that combines hard boundary condition imposition and adaptive weight tuning to quickly reflect the observed data while imposing the prescribed boundary conditions. The high reliability and efficiency of the presented method is verified by numerical examples.

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Advanced numerical methods for the modeling and optimization of coupled dynamical systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ABOUT THE HUMAN-STRUCTURE INTERACTION THROUGH A SELF-EXCITED SPRING-MASS-DAMPING MODEL ON RECTANGULAR PLATES

Zenon Del Prado[*1] and Phablo Dias*[1]

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ABSTRACT

In this study, the human-structure interaction during jumping on a thin rectangular plate is examined. The rectangular plate is modeled according to the nonlinear theory of Von Karman, exploring various boundary conditions and geometric imperfections to closely simulate real behavior of building floors structures. To describe the human effect on the plate, initially, a self-excited single-degree-of-freedom Mass-Spring-Damper (SMD) oscillator is used. Subsequently, a second SMD oscillator is introduced to assess the effect of the synchronism of rhythmic jumping by two jumpers on the plate. A detailed parametric analysis is conducted using the theory of smooth contact dynamics to examine the influence of contact loss during the flight phase of jump cycles. The dynamic response of the plate is analyzed for different values of human biodynamic factors, such as human damping ratio, and the frequency and amplitude of jumps. Consequently, the human response to these changes is evaluated.

ANALYSIS OF WAVEGUIDE PROBLEMS WITH IMPEDANCE BOUNDARY CONDITIONS

Leszek Demkowicz[*1], *Norbert Heuer*[2] *and Jay Gopalakrishnan*[3]

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[2]*Catholic University of Chile*
[3]*Portland State University*

ABSTRACT

The presented work is motivated with the well-posedness analysis for bent optical fibers. To our best knowledge, even the simplest 2D model acoustical waveguide problem in polar coordinates with an impedance boundary condition remains an open problem. We will present at least results for the related straight waveguide problem. Similar to the standard problem with hard boundary conditions, the L^2 stability constant for the first order system depends linearly upon the waveguide length L. The proof is based on the classical (but little known) theory for non self-adjoint operators, see [1]. The results are critical for the numerical analysis of bent optical fibers using the Discontinuous Petrov Galerkin (DPG) method.

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Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NONLINEAR OPTIMAL CONTROL FRAMEWORK FOR THE DPG METHOD

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ABSTRACT

The Discontinuous Petrov-Galerkin (DPG) method is a novel technology to solve partial differential equations numerically, and has been developing rapidly and applied to a broad range of problems in the past 15 years. As a minimum-residual method, the DPG method comes with guaranteed discrete stability and a-posteriori error estimator, which can be utilized to drive hp-adaptive refinements. The majority of applications of DPG involve linear problems; to tackle any nonlinear problem, we have to first linearize the problem, then apply the DPG method to the linearized problem. However, there is no easy guarantee that by minimizing the residual successively for every linearized problem, we obtain a residual minimizing solution of the nonlinear problem. Hence we consider the nonlinear optimization problem directly, in an optimal control framework [1]. As a standard technique in optimal control, we can compute the gradient by introducing the Lagrangian and solving the adjoint equation. With the gradient at hand, we can use steepest descent or nonlinear conjugate gradient methods (e.g. Polak-Ribière) to minimize the residual and obtain the final solution in an iterative way.

In contrast to [1], where Hessian-based methods are developed, we focus on gradient based methods, for two reasons. First, the problem we are interested in may involve cost functional which is not second order differentiable (e.g., penalty functional for inequality constraints). Second, apart from the test norm, the trial norm also enters the computation of the gradient. The freedom of choosing a trial norm means that we can get faster convergence by a wise choice. We analyze, in particular, the linear case, where we can get one-step convergence if the trial norm is the energy norm; if we use L2 trial norm and adjoint graph norm as test norm, linear convergence is also guaranteed, and we find explicitly an upper bound of the spectral radius.

Lastly we demonstrate the capability of our method by solving two nonlinear PDEs. The first problem is a manufactured one, and we compare our results with [2]. The second problem is the full-potential equation.

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Advanced materials: Computational analysis of properties and performance
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CONVERGENCE ANALYSIS AND ERROR ESTIMATION FOR MIXED FINITE ELEMENT METHOD MODELING FLEXOELECTRICITY

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ABSTRACT

Flexoelectricity is the coupling between strain gradient and electric field (or polarization) in dielectric materials under inhomogeneous deformation. The Mathematical framework describing flexoelectricity is a boundary value problem (BVP) governed by 4th-order partial differential equations (PDE). Direct modeling of the problem BVP with the use of the conforming Finite element method (FEM) requires C1-continuous elements that are complicated to construct and difficult to use. Mixed FEM is another practical approach and shows excellent potential in modeling flexoelectricity as it involves only C1-continuous finite elements. However, the convergence theory and error estimation formula for mixed FEM are absent up to now. In this work, we established a mixed variational principle for general flexoelectric problems by introducing displacement gradient as independent variables and confirmed the well-posedness of the variational principle. Following this, we developed several mixed finite elements that satisfy the well-known inf-sup condition.
Further, we estimated the error of numerical results from the exact solutions for primary and extra variables. In addition, numerical tests were conducted for several benchmark problems, and numerical results were performed in excellent agreement with the presented error estimation. This work bridged the gap of numerical analysis for mixed FEM in modeling flexoelectricity.

Advances in multi-scale, multi-material, and multi-component Topology Optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN DESIGN OF MULTISCALE NONLINEAR SPINODAL MATERIALS

Shiguang Deng[*1], Liwei Wang[1], Stefan Knapik[1], Horacio Espinosa[1] and Wei Chen[1]*

[1]Northwestern University

ABSTRACT

In recent years, there has been significant research interest in bio-inspired spinodal metamaterials. This is attributed to their versatile and nonperiodic structure, which is less sensitive to manufacturing defects, stress concentration, and material failure compared to conventional materials. However, the design and optimization of such spinodoids often face challenges due to the vast design space of microstructural morphology. Existing efforts have primarily focused on quasi-static linear elastic loading scenarios, neglecting the material's significant potential for nonlinearity. This oversight is attributed to the high costs associated with nonlinear analyses and the laborious derivation of nonlinear sensitivities.

In our work, we introduce a data-driven multiscale topology optimization method that combines microscale spinodal optimization with macrostructural topological design in a generic neural network (NN) framework. Specifically, we formulate a controlled anisotropy scheme in the spectrum density function to accurately depict stochastic, non-periodic, and amorphous microstructures using only a handful of design parameters in a low-dimensional design space. In addition, to emulate the material nonlinearity of hyper-elastically behaved spinodoids subject to large deformation, we employ Gaussian Process (GP) models to establish correlations among material geometry, strain, and stress states. Subsequently, we incorporate the GP models into the NN-based multiscale topology optimization where the tedious derivation of nonlinear sensitivity (which is often performed manually) is seamlessly replaced by NN’s automatic differentiation functionality. To demonstrate the proposed method, we present numerous examples that highlight the superiority of our multiscale spinodal design over conventional multiscale truss-like structures, especially in nonlinear applications.

Scientific machine learning for geophysical applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RC-CAN: RANGE-DEPENDENT CONDITIONAL CONVOLUTIONAL AUTOENCODER FOR REAL-TIME FAR-FIELD UNDERWATER NOISE PREDICTION

Indu Kant Deo[*1], Akash Venkateshwaran[1] and Rajeev Jaiman[1]*

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ABSTRACT

The transmission of underwater noise in the ocean is an intricate and dynamic process influenced by the complex geometry of ocean bathymetry. Developing accurate and general physical models for predicting acoustic transmission loss in diverse oceanic conditions has been a longstanding challenge. In addressing this challenge, we introduce a novel solution called the Range-Dependent Conditional Convolutional Autoencoder Network (RC-CAN), a deep learning model specifically designed for the real-time prediction of far-field underwater acoustic noise in varying bathymetry ocean environments.

Being data-driven, the RC-CAN model offers a unique advantage, relying solely on data irrespective of the method of data acquisition. By learning a latent representation of input ocean geometry, RC-CAN efficiently reconstructs distributions of far-field transmission loss across the provided ocean mesh. We evaluate the RC-CAN model in a two-dimensional ocean environment with varying bathymetry specifically on the benchmark test case of Dickin's Seamount, revealing its exceptional ability to learn fundamental factors influencing acoustic signal transmission loss, such as sound wave spreading, refraction, and reflection from ocean surfaces and floors. RC-CAN's capacity to capture the intricacies of ocean acoustics holds tremendous potential for real-time prediction of far-field underwater noise. The versatility of our framework suggests its potential applicability in predicting large-scale 3D underwater radiated noise. This innovation could revolutionize decision-making for marine vessels and online control strategies, enabling informed and timely interventions in the constantly changing underwater auditory environment.

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Advanced computational modelling of wood, wood-based products, bio-composites, and timber structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MOLECULAR DYNAMICS STUDY OF THE HYGRO-MECHANICAL BEHAVIOUR OF NATURAL AND CONSOLIDATED WOOD

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ABSTRACT

To better understand the hygro-mechanical behaviour of wood, Molecular Dynamics combined with Grand Canonical Monte Carlo simulations [1] is used to model sorption and sorption-induced deformation and determine the mechanical properties of wood components and their mixtures. Adsorption or desorption of moisture are modelled with an imposed chemical potential during the GCMC simulation, while deformation, either swelling or shrinkage, are modeled under constant pressure in MD. In our study, GCMC is implemented using Cassandra package and MD is performed using GROMACS. In this study, we analyze the hygromechanical behavior of amorphous cellulose (AC), mimicking a natural wood component, and of the mixture of AC and polyethylene glycol (PEG), where PEG is used to consolidate.

The results show that pure AC is a hygroscopic material, showing a substantial swelling-induced sorption and a mechanical weakening upon sorption. It also shows hysteresis between adsorption and desorption isotherms. Pure PEG shows much higher moisture contents and swelling strains at high relative humidity (RH) compared to AC, what opens the question how PEG can reduce AC's sorption behaviour. Our results confirm that adding PEG reduces the sorption and swelling behaviour of AC. This counterintuitive observation can be explained by: (1) PEG fills a large part of the existing porosity in AC, as such preventing additional sorption; (2) PEG molecules are constrained by the existing AC structure, hindering swelling and additional swelling-induced sorption. PEG is also found to weaken the material structure reducing the mechanical stiffness. A poromechanical model is developed describing the hygromechanical behaviour of AC, PEG and AC+PEG mixtures allowing to optimize the consolidation process, showing an optimal PEG mass fraction of 15%.

This study was inspired by the treatment of waterlogged archaeological wood of shipwrecks, like the Varsa and Mary Rose, with PEG for its consolidation and stabilization, where PEG molecules replace the water making wood at museum conditions less susceptible to changes in humidity and able to sustain mechanical load.

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Multi-physics and multi-scale simulations with the coupling library preCICE
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MICRO MANAGER: A TOOL FOR MULTISCALE COUPLING WITH PRECICE

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ABSTRACT

For many challenging applications in simulation technology, micro-scale phenomena can dominate macro-scale behavior. Examples in this setting are reactive porous-media flow, biomechanical models of the human organs, and composite structures. This talk presents a novel software framework to couple existing micro-scale and macro-scale simulations in an adaptive and flexible way. We present the Micro Manager, a software component which manages a set of micro simulations, and couples them to the macro simulation through preCICE. By design, preCICE is able to couple two or more models on one physical scale. Hence, we develop the Micro Manager, to allow for application-agnostic macro-micro coupling with preCICE. While reusing key coupling implementations of preCICE (e.g., parallel communication and fixed-point acceleration schemes), the Micro Manager calls all micro-scale simulations as libraries in an adaptive manner and is itself coupled to the macro-scale simulation using preCICE. We show several applications which use the Micro Manager. For every case, we investigate running the micro simulations adaptively, and its effect on load balancing for large parallel cases. Lastly, we present a dynamic load balancing strategy to increase efficiency of large cases.

Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LÉVY'S SOLUTION FOR LAMINATED COMPOSITE PLATES USING HIGHER-ORDER SHEAR AND NORMAL DEFORMATION THEORY

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ABSTRACT

Equivalent single layer theories (ESL) have been extensively used in the analysis of plates. One of the common assumptions that are considered in all the ESL theories is that the thickness is small as compared to the in-plane dimensions. This assumption is the basis for converting a 3D plate problem into a 2D plate problem by assuming a displacement-model along the thickness. Higher-order shear deformation theories (HOSTs) consider more realistic non-linear variation of displacements along the thickness as compared to the other ESL theories i.e., the classical plate theory (CPT) and first-order shear deformation theories (FOSTs), which consider the linear variation. Due to this reason the solutions obtained using HOSTs are closer to the elasticity solutions. In this paper, static solution of the laminated composite plates is provided using 12 degrees of freedom higher-order shear and normal deformation theory (HOSNT). Results are obtained using the state-space approach for Lévy-type plates i.e., two opposite plate edges having simply-supported boundary condition and other two plate edges having combination of simply-supported, clamped and free boundary conditions. Results from the work compare well with the corresponding results available in the literature. Model can be used for accurate and expeditious analyses of laminated composite as well as sandwich plates.

SEMICLASSICAL NUMERICAL MODELING OF GAIN MATERIALS WITH A HIGH ORDER DISCONTINUOUS GALERKIN TIME-DOMAIN SOLVER

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ABSTRACT

In this talk we discuss numerical modeling of the interaction between an electromagnetic field and a gain medium in the context of laser physics, with the goal of simulating the gain process that results in an increase in optical power. This phenomenon can be modelled by a four-level atomic differential system that
couples Maxwell’s equations with a set of non-linear Ordinary Differential Equations to describe the electronic density evolution for each energy level. We present a novel numerical modeling leveraging a Discontinuous Galerkin Time-Domain method in 3D, this method is validated in a 3D framework using a model problem with manufactured solution and is used in more realistic problems.

Mechanobiology of cells, vesicles and biomembranes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOWARDS PREDICTING RAFT COALESCENCE AND NUCLEATION INDUCED BY LIGAND-BINDING ACROSS THE CELL MEMBRANE

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ABSTRACT

This current paper studies lipid rafts co-localization during ligand-binding triggered by chemically affine transmembrane receptors (e.g. GPCRs-G Protein Coupled receptors). The latter populate the cell membrane and respond to external ligands through signaling producing cAMP-cyclic Adenosine Mono Phosphate. This is known to be the final product of a cascade of events triggered by activated GPCRs through their conformational changes and simultaneous membrane remodeling. Such activation is mediated by evolving raft co-localization as GPCRs find the right environment for their activation precisely on those sites [1]. Homeostatic levels of cAMP are known to be maintained over time thanks to the presence of MRPs-Multidrug Resistant Proteins, which play the role of signaling regulators in such dynamics. Due to the 'confining' work that the active species exert on the surrounding lipid clusters, the interspecific kinetics between GPCRs and MRPs, and their diffusion across the membrane, are coupled with the deformation of the hosting membrane, at is was found in [2]. In such a paper rafts formation was predicted to be triggered by ligand-receptor activity across the membrane.
Unfortunately, that work provided no insights into the experimentally observed raft coalescence. This is analyzed here through a Cahn-Hilliard type energetics and kinetics of the phase transition of both GPCRs and MRPs. The resulting chemical potential for each species is determined by the change in this newly determined energy plus the specific confining work mentioned above. The interplay between the balance of forces and coupled interspecific kinetics shows diffusive-induced membrane remodeling and raft coalescence, enhancing the size of active receptor sites. Sensitivity analysis suggests how such outcomes can predict cell membrane changes and remodeling by keeping track of active species near homeostasis and, also, away from such states [3].
This could help to gain new insights into the remodeling of cell membranes and could suggest mechanically based strategies to control their selectivity, by orienting intracellular functions and mechanotransduction.

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Multiscale modeling of dynamics in complex media and metamaterials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BOUNDS ON Q-FACTOR OF QUASI-STATIC METAMATERIALS AND OPTIMAL MICROSTRUCTURE DESIGNS

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ABSTRACT

Resonances in materials have led to many exciting properties and applications in nano-photonics and optics.
A famous example of material resonance is the "Lycurgus cup", which is a 4th century Roman drinking cup made of glass with fine particles of gold suspended in it. The resonances of the gold particles at optical wavelengths cause it to appear either red or green depending on where the light shines from. By making the gold particles hollow one can shift the resonant frequency, even into the infrared where nanoshells have proved significant in destroying cancer cells. So, it is of great interest to know what are the limits to which they can be tuned. The bandwidth of the resonances in materials is an important feature which is commonly characterized by using the Q-factor. We present tight bounds correlating the peak absorption with the Q-factor of two-phase quasi-static metamaterials and plasmonic resonators evaluated at a given peak frequency by introducing an alternative definition for the Q-factor in terms of the complex effective permittivity of the composite material. This composite may consist of well-separated clusters of plasmonic particles and thus we obtain bounds on the response of a single cluster as governed by the polarizability. Optimal metamaterial microstructure designs achieving points on the bounds are presented. The most interesting optimal microstructure is a limiting case of doubly coated ellipsoids that attains points on the lower bound. We also obtain bounds on Q for three dimensional, isotropic, and fixed volume fraction two-phase quasi-static metamaterials and particle clusters with an isotropic polarizability. Some almost optimal isotropic microstructure geometries are identified.

Advanced materials: Computational analysis of properties and performance
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STATISTICAL INVESTIGATION OF THE FAILURE MODES OF STRUT BENDING AND COMPRESSION DURING COMPRESSION LOADING OF POLYDISPERSE CERAMIC FOAMS

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ABSTRACT

The work studies the modes of failure of the struts during uniaxial compression loading of a ceramic foam with polydisperse pores. The foam is made by mechanical stirring of an alumina slurry [1]. Its microstructure resembles interconnecting polydisperse pores. Gibson-Ashby [2] models (GA) correlate the uniaxial compression failure of open-cell foam to the bending failure of its struts. The strut thickness increases with the relative density and beyond a certain density, the failure mode changes to strut compression and the material no longer resembles a foam. This understanding works well in the case of foams with monodisperse pores. However, in foams with polydisperse pores, there is a wide distribution in strut thickness and orientation for a constant value of relative density. This study answers the question of whether this leads to a combination of failure modes in which strut bending and strut compression act together to cause macroscopic failure. For this, a novel image segmentation algorithm is developed to isolate the struts in the foam microstructure obtained by micro-CT scanning [1]. The distribution of strut thickness and orientation is quantified. Next, a finite element-based uniaxial compression simulation is performed on the same microstructure to identify the failure modes of the struts. It is seen that strut failure mode depends on its thickness and orientation with respect to the loading direction. Classifying the type of strut failure at each step of the loading curve shows that the struts oriented normal to the load direction fail in bending at the very early stages of the loading. However, the macroscopic load keeps on increasing as the struts orientated parallel to the loading are in compression and withstand more load since the compression strength of the base material is much higher than the tensile strength. Macroscopic failure occurs when these struts fail in compression. The numerical value of the compression strength agrees well with the experimental value [1]. Since the dominant mode of strut failure is compression, the strength value is higher than the prediction by the GA open-cell model which assumes strut bending as the failure mode. These conclusions necessitate the development of better models to predict compression failure of such foams that will take into account both failure modes of the struts.

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Advanced simulation techniques for the structural design of carbon reinforced concrete
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

POSSIBILITIES FOR NUMERICAL MODEL VALIDATION THROUGH COMPUTED TOMOGRAPHY GENERATED DATA

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ABSTRACT

In order to make accurate predictions of the structural behaviour of FRP reinforced concrete elements, one of the key problems in the development of this type of new material system is the capacity of modelling the load transfer mechanisms between the concrete matrix and the reinforcement elements. To predict the load-deflection response up to ultimate limit state conditions, a wide range of numerical simulation approaches, with capability of modelling the bond behaviour between the different materials have been proposed over the years and compared to experimental results. This research work presents new possibilities for comparing numerical finite elements models (FEM) with laboratory data generated by computed tomography, namely in the context of three point bending tests performed on carbon-reinforced concrete specimens. The aim is to validate numerical simulation results through computed tomography generated data. Examples of possible validation procedures are shown, which focus on generated strain fields and crack patterns.

Advanced discretization schemes and solution strategies for computational structural dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A COMPARATIVE STUDY OF ADAPTIVE IMPLICIT-EXPLICIT AND EXPLICIT-EXPLICIT TIME-MARCHING PROCEDURES FOR WAVE PROPAGATION ANALYSES

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ABSTRACT

This paper delves into the effectiveness of two time-integration techniques, namely the adaptive implicit-explicit (imp-exp) and explicit-explicit (exp-exp) methods, which stand as efficient formulations to address complex systems with multiple time scales. The imp-exp technique blends implicit and explicit procedures, automatically applying implicit and explicit elements for the faster and slower components of the considered model, respectively. Interface conditions do not need be considered in this hybrid approach, rendering a very straightforward technique. In addition, it enables to compute the most favorable time-step value for optimal performance considering implicit and explicit sub-domains distribution, providing an entirely automated highly effective formulation. On the other hand, the exp-exp method, a variant of the considered explicit approach incorporating sub-cycling, employs smaller sub-steps to address the faster elements of the model. In this case, different time-step sub-domains are automatically distributed along the model, following the stability conditions of the referred explicit approach and the properties of the discretized model, enabling larger time-step values to be properly locally applied and enhanced analyses provided. Both these multi-domain techniques provide adaptive algorithmic dissipation, allowing for the local application of numerical damping if necessary, according to the properties of the adopted discrete model and its computed responses. Numerical results are presented at the end of this manuscript, illustrating the good performances of these adaptive procedures, as well as discussing the circumstances under which one approach should be favored over the other, providing valuable insights for decision-making in practical implementations. Special emphasis is placed on geophysical applications exhibiting multiscale configurations.

Numerical modelling of composite materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL ANALYSIS OF A FRCM-STRENGTHENED MASONRY COLUMN SUBJECTED TO COMPOSITE DEBONDING

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ABSTRACT

In recent years, there has been a growing focus on a new generation of fiber-based strengthening systems, specifically Fabric Reinforced Cementitious Matrix (FRCM). While Fibre Reinforced Polymers (FRP) are widely acknowledged for their effectiveness in retrofitting interventions, the preference for new composite materials with an inorganic matrix is often attributed to their greater reversibility and compatibility with historical architectural heritage.

The potential of FRCM in enhancing the structural performance of reinforced concrete structures has been demonstrated by numerous studies, whereas the literature studies focusing on masonry and historical buildings is inadequate due to the heterogeneity, complexity and aleatory nature of the material. Due to the abovementioned limited applications/studies, numerical models and simulations of masonry structures retrofitted with FRCM remain an open issue, especially with regard to the interactions between the inorganic matrix and reinforcing fibres.

This study implements a 3D Finite Element (FE) analysis of a small-scale masonry column retrofitted by FRCM reinforcement and subjected to tensile (debonding) loading within the reinforcement layer; the analysis is carried out in ABAQUS. The case study is derived from an experimental study [1]. The retrofitted column is modelled using a micro-modeling approach, developed according to the latest literature advances [2]. Each material is individually modelled and assigned its mechanical characteristics, calibrated based on past experimental data; two fictitious surfaces are introduced to simulate the nonlinear interaction between the inorganic matrix layer and the reinforcing fibres and to investigate the global bond behaviour. The numerical results are compared with the reference experimental outcomes both in terms of load-displacement curves and damage evolution, and the comparison shows a good agreement. Accordingly, the modelling approach can be efficiently extended to further case studies not experimentally assessed.

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Advance and application of meshfree methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMMERSED B-SPLINE FOR IMPROVED THE IMPOSITION OF ESSENTIAL BOUNDARY CONDITIONS IN THE MATERIAL POINT METHOD

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ABSTRACT

The Material Point Method (MPM) is a particle based method in which solids or fluids are discretized into a series of points. These points move freely through a computation background grid that spans the whole physical domain. Through the discretization process, knowledge of where the boundaries lie is lost. This is problematic for the imposition of essential boundary conditions. In some limited cases, the boundaries onto which these conditions need to be applied coincide with the background grid nodes. In these cases, the imposition is directly done via the background grid. However, in most cases, this is not possible.

This problem is not specific to the Material Point Method but to all particle based methods and also to cutFEM. In cutFEM, the finite element mesh can cut through the solid domain, again making the imposition of essential boundary conditions difficult. In this context, Sanchez et al. (10.1016/j.cma.2010.12.008) have developed the Immersed B-splines that are a modification of the standard B-splines shape functions to locally interpolate exactly the Dirichlet boundary conditions.

B-spline shape functions are already commonly used in the MPM to mitigate stress oscillations due to points crossing background grid cells. Immersed B-splines are regular B-splines that are modified such that their support outside of the solid or fluid domain is null, exact on the boundaries and identical to standard B-splines in the bulk. This way, boundaries can be tracked and Dirichlet boundary conditions can be applied to the background grid easily, independently of the position of the solids or fluids with respect to it.

In this work, we adapt the Immersed B-splines to the Material Point Method and demonstrate with 2D and 3D examples the efficiency and robustness of the proposed approach to simulate large deformation problems with imposed non-trivial Dirichlet boundary conditions.

Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A PRIMAL HYBRID FINITE ELEMENT METHOD TO SOLVE GENERAL COMPRESSIBLE, QUASI-INCOMPRESSIBLE AND INCOMPRESSIBLE ELASTICITY USING STABLE H(DIV)-L2 SPACES

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ABSTRACT

Hybrid methods are usually derived from an extended variational principle, in which the interelement continuity of the functions subspace is removed and weakly enforced by means of a Lagrange multiplier. In this context, a new primal hybrid finite element formulation is presented, which uses H(div) conforming displacement functions and discontinuos L2 approximation for pressure together with shear traction functions to weakly enforce tangential displacement. This combination allows the simulation of compressible, quasi-incompressible and fully incompressible elastic solids, with convergence rates independent of its bulk modulus. The proposed approach benefits from the property that the divergence of the H(div) displacement functions is De Rham compatible with the (dual) pressure functions. The hybridization of the tangential displacements is weakly enforced through a lower order shear stress space. This leads to a saddle-point problem that is stable over the full range of poisson coefficient (large compressibility up to incompressible). Moreover, a boundary stress (normal and shear) can be recovered that satisfies elementwise equilibrium. Hybridizing the tangent stresses and condensing the internal degrees of freedom, a positive-definite matrix with improved spectral properties can be recovered. The stability, consistency and local conservation features are discussed in details. The formulation is tested and verified for different test cases.

ON THE ITERATIVE SOLUTION OF SADDLE POINT PROBLEMS USING A SYMMETRIC POSITIVE DEFINITE PRECONDITIONER

Philippe Devloo[*1], Giovane Avancini[2] and Marina Meneghel[2]*

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ABSTRACT

Saddle point problems frequently appear in many mathematical and engineering applications. Most systems of partial differential equations with constraints give rise to saddle point linear systems. Typical examples include mixed finite element formulations to solve fluid flows and/or elasticity problems under full incompressibility. The inversion of saddle point problems is challenging due to inherent numerical instability in the direct inversion methods. Many direct and iterative methods have been proposed to overcome this challenges, such as the Schur complement and the Uzawa's method. In the context of mixed finite element for incompressible flows using stable H(div)-L2 spaces for velocity and pressure, we propose an iterative method that can effectively solve a saddle point problem iteratively by summing a small compressibility to the original matrix. The preconditioning matrix is symmetric positive-definite, which allows the usage of Cholesky decomposition and/or CG-like iterative solvers to compute the incremental solution for the velocities unknowns. A procedure to compute the average pressure of each element of the incompressible problem is developed using the unbalanced fluxes caused by the compressibility perturbation. The average is updated during the iterative process as a function of the velocity increment at each iteration.

Modeling and simulation of advanced manufacturing processes for metals
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

REAL-TIME ESTIMATION OF THERMOMECHANICAL STATE DURING ADDITIVE MANUFACTURING BY ASSIMILATING INFRARED IMAGING DATA INTO SIMULATIONS

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ABSTRACT

Additive manufacturing techniques for metal alloys are revolutionizing product design and manufacturing. However, suboptimal process parameters and stochastic aspects of printing can lead to significant variability in component quality, making qualification and deployment difficult. The ability to comprehensively monitor the printing process is vital to ensure that a particular component is usable and can provide valuable clues as to how the process can be modified to limit adverse results.

Many modes of in-situ monitoring have been demonstrated, with thermocouples and imaging at visible and infrared (IR) wavelengths being most widely used [1]. However, these methods have a significant drawback – they cannot create a full 3D reconstruction of the thermomechanical state. Instead, they give a limited view of quantities along non-blocked exterior surfaces (imaging) or at individual points (thermocouples). 3D characterization is possible with x-ray and neutron diffraction, but these require large facilities that are not tractable for practical manufacturing settings. An estimate of the full 3D thermomechanical state is important because thermal gradients that lead to residual stress and other quantities of interest usually vary dramatically throughout the interior of the part being printed.

We demonstrate a method to estimate the full 3D state in real-time by incorporating in-situ observations from imaging and thermocouples into faster-than-real-time thermomechanical simulations. We achieve this via an ensemble Kalman filter, an approach widely used in the meteorological community. Recently, Wood et al. [2] demonstrated the use of an ensemble Kalman filter for additive manufacturing, albeit with synthetic “experimental” data from a simulation. In this presentation we show the application of an ensemble Kalman filter using real experimental data from IR cameras and thermocouples from a directed energy deposition (DED) experiment. Our contributions are four-fold: 1) a flexible pipeline to collect, analyze, and transport in-situ characterization data, 2) raytracing capabilities to map image pixels to locations on a finite element mesh, 3) a performant finite element code that permits faster-than-real-time component-scale calculations, 4) a ensemble Kalman filter implementation that is tightly integrated into the finite element simulation software.

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Architected materials and structures
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COMPUTATIONAL MODELING OF MEMBRANE TENSEGRITY STRUCTURES

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ABSTRACT

Traditional tensegrity structures are spatial structures with strings in tension isolating struts in compression, together providing the necessary structural resistance to loads. These structures have found diverse applications in aerospace, structural, programmable matter, and soft robotics. Recently, there has been a growing interest in membrane-tensegrity structures, which are two-dimensional analogs with compressible elements (rods) embedded in a thin membrane. Here, the rods are in compression, isolated from each other, and are held in equilibrium by the tension in the membrane. These structures combine the advantages of lightweight and tailorability of traditional tensegrity with advantages of enclosed volume. Hence, such structures have found application in lightweight architectural domes [1,2]. Beyond civilian applications, these structures can potentially transform the frontiers of programmable material by integrating phase-transforming materials, sensors, and actuators. However, such expansion is not possible without computational tools for architecture-property prediction tools, which are currently absent.

This presentation presents a thin-shell computational model to study such systems. The membrane is modeled as a two-dimensional surface and links as elastic rods embedded in the membrane. We use a thin-shell finite element framework to compute the equilibrium configurations. Through a combination of computations and experiments, we will explore the subtle equilibrium landscape of this system, including the possibility of multi-stability.

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Computational modeling of extreme-loading events
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FAILURE UNDER IMPACT LOADING OF FOAM CORE IN SANDWICH STRUCTURES WITH FIBER-REINFORCED COMPOSITE FACE SHEETS

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ABSTRACT

We analyze transient deformations of a sandwich plate with glass fiber-reinforced vinyl ester composite face sheets and three layers of equal thickness of CorecellTM foam cores to delineate its deformations. The face sheet material is modeled as linearly elastic and transversely isotropic with the axis of transverse isotropy along the fiber. The damage is assumed to initiate at a point in a face sheet according to Hashin's failure criteria. The Matzenmiller et al.'s [1] approach is used for damage evolution and degrading the material elasticities. Bazant and Oh's [2] crack-band model that incorporates a material characteristic length into the analysis is adopted for deleting an element. The foam is modeled as an elastic-plastic material obeying the Johnson-Cook (JC) effective stress-effective plastic strain relation that accounts for strain-hardening, strain-rate hardening, damage induced softening, and assumes the material to be isotropic and plastic deformations to be isochoric. The failure is assumed to initiate at a critical value of the damage computed using the JC damage criterion. The material elasticities and the flow stress are then degraded to zero by specifying an effective plastic displacement. Elements with essentially negligible values of the elastic moduli and the flow stress are deleted from the analysis. The plastic strain component with the maximum magnitude is associated with the failure mode.
Values of foam parameters in the JC relation are identified by using the experimental axial stress–axial strain curves included in Wang et al. [3]. The numerical solution of the problem by the finite element method based software, Abaqus, is found to qualitatively compare well with test findings [3]. However, the two quantitatively differ somewhat that can partially be attributed to neglecting in the analysis the anisotropy of the foam, uncertainties in values of its parameters found by using the axial stress – the axial strain data, assuming plastic deformations of the foam to be isochoric, and discrepancies in the experimental and simulated boundary conditions and the loads applied.

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Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPOSABLE DESIGN OF MULTIPHASE FLUID DYNAMICS SOLVERS IN FLASH-X

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ABSTRACT

Multiphysics fluid dynamics simulations play a crucial role in understanding and predicting the intricate behaviors of complex engineering systems. Numerical modeling of interactions among solids, fluids, and multiple phases, such as liquid and gas, has generated significant research interest in recent decades. This has led to the development of open-source simulation tools and commercial software products targeting specific applications or general problem classes in computational fluid dynamics. As the demand increases for these simulations to adapt to platform heterogeneity, ensure composability between different physics models, and effectively utilize inheritance within partial differentiation systems, a fundamental reconsideration of numerical solver design becomes imperative. To address these challenges, we will present our work on Flash-X (https://flash-x.org), as a potential solution. The software design strategies that we employ can serve as a guide, offering insights into navigating the intricate terrain of performance portability, composability, and sustainable development. We will demonstrate how generative AI can be leveraged to improve design of both new and existing simulation tools grappling with these challenges. By incorporating the principles outlined in the Flash-X approach, engineers and researchers can enhance the adaptability, efficiency, and overall effectiveness of their numerical solvers in the ever-evolving field of multiphysics simulations.

Multiphase flow and non-Newtonian fluid - Modelling and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE BREAKING OF THREE-DIMENSIONAL WAVES

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ABSTRACT

The breaking of ocean waves contributes significantly to wave energy dissipation and marks the transition from laminar flow to turbulent mixing at smaller scales on the ocean surface. The implications of wave breaking extend to particle transport, influencing the fate of oil spills and plastic pollutants.

Numerical codes for the computation of water waves must include breaking criteria and models for energy dissipation in order to accurately predict water surface changes, energy loss, and turbulence. Numerous onset criteria have been proposed over the past seven decades, through theoretical studies, numerical simulations, laboratory experiments, and field observations.

Measuring the properties of 3D waves, especially breaking and near-breaking waves, presents challenges due to their steepness, rapid spatial variations, and the technical difficulties in accessing turbulent flow fields and size distributions of drops and bubbles during active breaking times.
Recent advancements in computational capacity and numerical methods have made three-dimensional Direct Numerical Simulations (DNS) of breaking waves feasible, providing an appealing tool without the need for parameterizations. These simulations allow for the investigation of the three-dimensional two-phase flow dynamics from initiation to post-breaking, and have shown reasonable agreement with available laboratory data.

We perform direct numerical simulations for the breaking of the simplest non-trivial three-dimensional waves: The short-crested wave system, defined as doubly periodic waves in the plane. This wave system, more prevalent in nature than its two-dimensional counterparts on complex oceanic surfaces, is generated within a wind fetch, from intersecting swell waves, or leeward of offshore islands or structures due to diffracted wave interactions.

In addition to the controlling parameters of the breaking waves of two-dimensional waves which exhibit regularity in terms of their crests, we investigate the effect of the wave obliquity on the breaking onset dynamics through some of the commonly used geometrical and kinematic criteria. We also analyze its impact on energy dissipation and post-breaking processes.

Architected materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DAMAGE PROPAGATION IN ARCHITECTED MATERIALS

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ABSTRACT

In this study, we explore fracture propagation within a two-dimensional Maxwell lattice. Traditionally, elastic brittle materials undergo catastrophic failure due to stress concentrations at crack tips. Maxwell lattices, operating at the brink of mechanical stability, offer an avenue to manipulate damage propagation and mitigate defects. We elucidate the underlying principles governing fracture control in a kagome lattice and demonstrate their application in engineering fracture paths within the lattice. Lattices are modelled as networks of sites interconnected by harmonic springs exhibiting elastic brittle behaviour. Our findings demonstrate the efficacy of these principles in governing crack behaviour and consequently enhancing the fracture toughness of the lattice.

Modern structure-preserving methods for PDEs
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGICAL METHODS FOR MODEL ORDER REDUCTION FOR SCALAR TRANSPORT EQUATIONS

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ABSTRACT

It is well-known [1] that proper orthogonal decomposition is not the most appropriate model order reduction (MOR) approach for hyperbolic problems. An alternative approach was proposed in [1] which uses L1 residual minimization over a solution dictionary to advance a solution forward in time from an initial condition. Success of this approach depends on the ability to find a small enough dictionary of solutions that captures the underlying dynamics.

Our previous work [2] demonstrated that the methods of computational topology [3], can be applied to reduce the dictionary size offline before solving the L1 minimization problem. In so doing we were able to reduce the computational cost of the L1 optimization problem, which was key to being able to obtain an effective reduced order model (ROM) for a model scalar transport equation.

We extend this work by demonstrating that in certain cases, one can estimate proto-basis functions, that can be refined into feasible basis functions for reduced order models, in 1 and 2 dimensional problems. Our approach is to use generators from persistent homology computed on spatial modes of an initial set of solutions to the model transport equation, which are optimal in terms of having a minimum size or measure. We then reconstruct the original dictionary elements as linear combinations of the topological basis functions and seek the solution of our model problem by interpolation between these sets of coefficients, followed by L1 minimization. We also will describe some recent enhancements to the L1 optimization procedure in terms of speed and stability.

This work will showcase the nascent fruits of an innovative and ambitious new effort for approaching reduced order models for hyperbolic systems which involves a largely unexplored application of algebraic topology to this problem domain.

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Advances in material model calibration for computational solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICS-INFORMED NEURAL NETWORKS FOR MATERIAL PARAMETER IDENTIFICATION IN QUASI-REAL PROBLEMS

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ABSTRACT

Physics-Informed Neural Networks (PINNs) have emerged as a promising approach for solving scientific and engineering problems that involve partial differential equations or physical constraints. PINNs are a type of Neural Network (NN) that incorporates physical laws or governing equations into its learning process. By combining the strengths of deep learning and physics-based modeling, PINNs can learn complex patterns and relationships from data while simultaneously satisfying the physics of the problem.

In this work, we explore the capabilities of PINNs to solve physical problems while identify material properties simultaneously. The validation example is a three-dimensional rectangular prism with a Neo-Hookean material, submitted to a compressive load. In this example, the estimated parameters were the first and second Lame's parameters. The reliability of the results was assessed by comparing them against the ground truth displacement data, which were obtained from the analytical solution. These values were used as input to evaluate the loss data function, while the remaining loss functions were derived from the physics of the problem.

With this validated PINN, two more realistic cases were studied. The first case attempts to simulate a simplified femoral cartilage, which is loaded with a known force, resulting in the deformation of the cartilage. The second case aims to simulate a breast undergoing compression in a mammography study, where the compression force is also known. Both cases were simulated using FEBio software to obtain displacements data.

The PINN, as implemented in the validation example, failed to accurately identify the material parameters for realistic cases. Consequently, the incorporation of new strategies into the PINN are studied. A loss function was implemented to balance the forces on the loaded faces based on the integral of the stress tensor. Additionally, independent networks were used for displacements and the parameters to be identified. Alongside this, a regularization loss function was implemented to incorporate prior knowledge about the material parameter constraints.

The results of this study suggest that PINNs have the potential to be an effective tool for both material identification problems and real-time prediction of the physical solution. However, it is important to note that further research and dedicated efforts are required to fully explore and harness the capabilities of PINNs in these domains.

CONTINUOUS DATA ASSIMILATION AND LONG-TIME ACCURACY IN A FEM FOR THE CAHN-HILLIARD EQUATION

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ABSTRACT

We propose a numerical approximation method for the Cahn-Hilliard equation that incorporates continuous data assimilation in order to achieve long-time accuracy and stability for arbitrarily inaccurate initial conditions provided enough data measurements are incorporated into the simulation. We conclude with a demonstration of the effectiveness of our method via several numerical experiments.

Computational and analytical advances in nonlocal modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE PERIDIGM MESHFREE PERIDYNAMICS CODE: MATHEMATICS, NUMERICS, AND COMPUTATION

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ABSTRACT

Peridigm [1] is a meshfree peridynamics code for use on large-scale parallel computers. It is an open-source, community driven software project. To date, Peridigm has been used primarily by methods developers focused on solid mechanics and material failure. This talk provides an overview of the mathematical models used in Peridigm and their numerical implementation, and demonstrates the use of Peridigm for practical computation.

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Towards predictive digital twins: Innovative algorithms for physics-, data-assisted and hybrid modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PATIENT-SPECIFIC ATHEROSCLEROTIC ANALYSIS SUPPORTING MEDICAL DECISION MAKING

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ABSTRACT

Geometries of arterial cross-sections are extremely diverse from patient to patient, as well as the distribution of their atherosclerotic plaque intrusions. Medical decision on whether a patient has low or high risk of rupture is made on the basis of this information, mostly of geometrical nature. Mechanical models analyzing stress distribution under internal pressure and the corresponding stress concentrations are of great help to support decision making. This is far of being integrated in clinical practice because the conversion of medical images into mechanical outputs of interest is a laborious process. The standard approach to tackle this problem consists in 1) processing the medical image into a segmented geometry, 2) to generate a compliant finite element mesh for the analysis, and 3) to solve the mechanical problem and compute the outputs of interest. Each of three steps is time demanding and jeopardizes the practical and translational use of these tools.

The aim of this research is to provide further tools allowing a seamless integration of the full process, minimizing the human intervention and providing robust and reliable computational outputs to support clinical decision making. First, an unfitted approach is devised for this specific case, allowing to encapsulate all the geometrical information in form of level sets supported in a background mesh to be used also in the computation of the mechanical problem. This presents the advantage of precluding the need of a constructing computational mesh, conformal with all the geometrical features of the section and its inclusions.

Moreover, this approach paves the way for a using Reduced Order Models (ROM) and therefore to drastically accelerate the computation. Nevertheless, the variability of the arterial cross-sections is a serious drawback for using ROM. The elements of the training set (snapshots) are too diverse to extract common features, and the new elements to be analyzed have little in common with the database from which the ROM has learned.

The work contributes to shape the mechanical problem statement with new boundary conditions, to provide insightful analysis of the dispersion of the observed different geometries, to devise a specific unfitted approach, and to test the ROM strategy in this scenario.

Advances in computational biomechanics and mechanobiology
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MESH MORPHING APPROACH TO ADDRESS THE EFFECT OF DEFORMABLE BOUNDARIES IN CFD SIMULATION OF AORTIC FLOW

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ABSTRACT

Altered local hemodynamics are recognized as a key contributor to aortic weakening leading to expansion and adverse outcome in aortic aneurysms. [1]. Computational fluid dynamic (CFD) simulations have been proposed as a clinical tool to stratify patients with respect to disease progression. However, as with most numerical simulations, these approaches require several assumptions including the velocity at inlet and outlet, the effect of external tissues, and the mechanical properties of the aorta and intraluminal thrombus [2]. To overcome these limitations, this study combines CFD on the fluid domain and structural analysis on the solid domain using a mesh morphing method [3] to prescribe displacement of the wall-blood interface directly to the numerical solver.
Four patients diagnosed with abdominal aortic aneurysm were included in the study. For each patient, strain on the aortic wall and on the lumen surface were obtained from pre-operative multi-phase CT scan. The changes in thickness of the thrombus were also computed to identify compression patterns within the thrombus. Nodes of the lumen surface mesh were defined as control points to use a radial basis function approach to morph the initial lumen geometry into each configuration throughout the cardiac cycle. The CFD simulation starts with a reference volumetric mesh that is replaced with isomorphic meshes at pre-defined time steps during the cardiac cycle. Two additional simulations were performed on the volumetric mesh at the diastolic and systolic configurations with rigid boundary conditions. Results from the simulations are compared in terms of time-averaged wall shear stress (TAWSS) and velocity streamlines at peak systole and diastole time points. Results show varying degree of difference between the rigid body and deformable wall simulations. Higher wall strain was associated with higher lumen displacements and resulted in greater difference between the moving wall and rigid simulations, suggesting that more accurate simulations can be obtained using this technique for patients with more deformable walls.
The dynamic mesh morphing technique to incorporate wall movement in CFD simulations enables more realistic and patient-specific simulation of aortic flow without introducing the uncertainty and computational cost that affect FSI simulations. The proposed technique could significantly improve CFD simulations, particularly for aortas with localized abnormal wall movement indicative of local weakening.

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Advances in computational mechanics for flow-induced vibrations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TURBULENT PIPE FLOW MANIPULATION USING TARGETED WALL SHAPES: A NEW TECHNOLOGY FOR ENERGY EXTRACTION

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ABSTRACT

Geothermal energy has become a leading alternative for energy supply to achieve near zero-emissions due to its high capacity factor. Wide-spread commercialization of geothermal energy harvesting technologies require advancements in efficient extraction of high-to-moderate temperature geothermal resources. To this end, we explored the development of a novel pipe-flow manipulation concept to lower frictional drag, increase extraction flow rate, and reduce heat losses to the ground formation. The flow manipulation is achieved through induced non-equilibrium wall-bounded turbulence using targeted wall shapes, as pre-placed inserts in fixed increments inside the geothermal pipe casing. The inserts adopt a shape of three-dimensional distinct azimuthal Fourier modes: m=3, 15, 3+15. In previous studies, a second-order pattern of recovery in turbulent flow was observed, which suggested long-lasting changes in flow properties. The studies further revealed the inserts achieve a maximum drag reduction of ~25% with the manipulated flow recovering to a regular state within 19D – 45D, depending on the wall-shape, at a range of Reynolds numbers, Re = 5×10^3 - 1.58 ×10^5. The behavior of axial gradient of peak mean velocity and turbulent kinetic energy downstream of the insert revealed that m=15 and 3+15 cases experienced a second-order response, while m=3 depicted a non-oscillatory trend. Using this information, the geometry was further modified by varying perturbation amplitudes and lengths to optimize the proven concept for commercial design. The oscillatory behavior of a perturbed flow is likely to cause vibrations and structural fatigue, making it important to investigate the fluid-structure interaction between the turbulent flow and pipe walls. We numerically modeled the altered geometries as incompressible pipe flows using an FSI-based solver in OpenFOAM. The FSI solver was implemented to investigate the turbulent flow-induced stress on the pipe, and to gain insight into the coupled fluid-structure effects of manipulated turbulent flow. The unsteady results will also provide us with critical design information regarding fatigue and structural vibrations induced by the flow manipulation. The performance of numerical models, along with the fluid and structural behavior, were assessed for design optimization. With its direct application to industry, this work holds importance in the field of renewable energy systems. Furthermore, this work expands our understanding of wall-bounded turbulent flow manipulation and FSI.

Catastrophic failure mechanics and numerical modelling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING ON THE MULTI-FIELD COUPLING DELAYED HYDRIDE CRACKING BEHAVIOR OF IRRADIATED ZIRCONIUM ALLOYS

Guochen Ding[*1], Zhongjia Xia[1], Jing Zhang[1] and Shurong Ding[1]*

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ABSTRACT

Zirconium alloys are widely used as the materials of nuclear cladding tubes or some other structural components due to their high strength, high corrosion resistance and low neutron absorption cross section. The chemical reaction between zirconium and coolant water in-reactor results in the absorption of hydrogen. Furthermore, the appearance of stress concentration facilitates the migration of hydrogen atoms towards the crack tip, which may induce delayed hydride cracking (DHC) and pose a potential threat to nuclear safety. In this study, an innovative multi-field coupling theoretical framework is formulated, integrating variables such as temperature, stress, damage factor, hydrogen concentration, hydride volume fraction, and hydride average orientation. To replicate the cracking process, a three-dimensional damage mechanical constitutive model, damage revolution model and the critical value of damage for damaged zirconium alloys are developed. The comprehensive model involves the effects of hydride-induced hardening and embrittlement, hydride orientation contributions and irradiation effect. In addition, a model for the irradiation-enhanced hydrogen diffusion coefficient is introduced to elucidate the influence of irradiation on hydrogen diffusion in zirconium alloys. Based on the differential governing equations for the concerned multi-field, the equivalent integral weak forms are derived for numerical implementation. The consistence between the predicted DHC velocities and experimental data, along with the representation of subcritical cracking traits, validates the effectiveness of the newly developed models. The irradiation-induced influence mechanisms for the delayed hydride cracking are analyzed and elucidated by the spatial distribution and evolution of multi-field results. This structured approach aims to provide a foundation for understanding the delayed hydride cracking behavior.

Design and mechanics of mutifunctional composites and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION METHOD OF LIGHTWEIGHT DAMPING COMPOSITE STRUCTURE

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ABSTRACT

Sandwich structures have the characteristics of high stiffness and light weight, and are widely used in aerospace, automotive, bridge, ship and other fields. Powder particle damper is a new type of damping structure based on additive manufacturing, which achieves damping by the collision energy loss between powders and between powder and the wall of damper. A concurrent topology optimization method for sandwich damping composite structure is proposed to improve the lightweight, load-bearing and damping performance, which includes stiffener layout, variable thickness skin and powder particle damper layout optimization. First, the damping characteristics and equivalent mechanical model of the powder particle damper are studied by experimental design and homogenization method; Secondly, the adaptive growth method based on the mechanism of biological branching system is adopted to optimize the layout of the stiffener rib. For structures with mass center position requirements, a mass center coordinate constraint technology is introduced. In order to further improve the damping performance and achieve lightweight of the structure, the concurrent topology optimization design of sandwich damping composite structure is carried out with the stiffener layout, variable thickness skin and powder particle damper position as design factors. Taking the rudder structure of high-speed aircraft as an example, the optimal design results shows that the vibration resistance performance of the structure is significantly improved while further reducing the structural weight. The proposed design method innovatively adopts the built-in powder particle damper as the damping means, combining the concurrent topology optimization of the stiffener layout and variable thickness skin, which provides a new approach for the design of sandwich damping composite structures.

Keywords: function-structure integrated design method, sandwich structure, powder particle damper, topology optimization, mass center constraint

Data-driven modeling and design of materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A UNIFIED SAMPLING AND LEARNING FRAMEWORK FOR TEXTILE-BASED METAMATERIALS

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ABSTRACT

Textile-based metamaterials have become widely used in engineering applications ranging from wearable sensors, health monitoring devices to soft robotics. The richness exhibited in their energy landscapes, which can be manipulated for desirable functionality, calls for a systematic sampling and learning framework. We propose a generalized parameterization to reconstruct 3D fibrous networks from 2D representative structures, assembled with varying local curvature and topology based on a yarn representation. This is a first step to enhance the data availability of textile-based metamaterials beyond conventional design. Using a first-principles computational model based on Lagrangian mechanics, we characterize their constitutive behavior through efficient sampling. We first show that a wide range of energy states can be explored from the process-structure-property mapping. Then, we facilitate the design of textile-based metamaterials to achieve tailored mechanical responses through machine learning techniques.

Recent advances on interfaces dynamics modeling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFECTS OF SURFACE ENERGY AND SUBSTRATE ON MODULUS DETERMINATION OF BIOLOGICAL FILMS BY SPHERICAL AND CONICAL INDENTATIONS

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ABSTRACT

Micro-/nano-indentation has become prevalent in evaluating the mechanical characteristics of biological samples, such as cells and tissues. However, the existing contact models describing conical indentation ignore the joint effects of surface energy and substrate, and consequently cannot accurately extract the Young's modulus of biological samples deposited on substrate. Through finite element methods, we examine the spherical and conical indentations of biological films on substrates while taking surface energy into account. Based on the dimensional analysis, the explicit relationship between load and indentation depth is achieved for films with their moduli varying from 0.001 to 100 times that of the substrate. If the classical contact models were employed to analyze the load-depth data, the modulus mismatch between film and underlying substrate would lead to an overestimation of modulus for the film on a stiffer substrate, but an underestimated modulus for that on a softer substrate. Meanwhile, in micro-/nano-indentations, neglecting the contribution of surface energy would result in an overestimation of the Young's modulus of films depending on the contact size. The analytical expressions provided here can be utilized to precisely deduce the mechanical characteristics of biological films deposited on substrate from the load and indentation depth data of indentations.

Mathematics and algorithms for predictive digital twins (DT)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DOMAIN DECOMPOSITION METHODS AND MODEL ORDER REDUCTION FOR PARAMETRIC LINEAR ELLIPTIC PROBLEMS

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ABSTRACT

Parametric partial differential equations arise in many computationally intensive applications like real-time computational design and optimisation. While model order reduction techniques provide an established methodology to effectively handle such problems, their computational cost still constitutes a bottleneck for problems involving many parameters and, possibly, multi-physics processes.
In this talk, we present a recent approach [1] that combines overlapping domain decomposition (DD) methods and proper generalized decomposition (PGD) to reduce the computational cost of constructing surrogate models for boundary value problems governed by linear parametric partial differential equations. The proposed methodology involves an offline phase where local surrogate models are computed by PGD, and an online phase where overlapping Schwarz DD methods are used to couple the local models, without the need to introduce Lagrange multipliers nor to solve any additional problems.
The application of the DD-PGD framework to the Stokes-Darcy problem to model the filtration of an incompressible fluid through a porous medium at low Reynolds number will be outlined. In this context, the suitability of adopting overlapping DD methods will be discussed both from a physical and a computational point of view [2,3].
Numerical results showing the effectiveness, accuracy and robustness of the proposed DD-PGD framework will be presented.

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Data-enhanced multi-model uncertainty quantification and experimental design of complex computational systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MULTI-FIDELITY STRATEGY FOR OPTIMIZATION UNDER UNCERTAINTY WITH ROBUST CONSTRAINTS

Thomas Dixon[*1] and Alex Gorodetsky*[1]

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ABSTRACT

Effective solutions for optimizing systems under uncertainty are crucial for ensuring the success of missions, enhancing the reliability of robotics, and preventing system failures. However, the conventional optimization under uncertainty approach often comes with substantial computational costs, making real-time implementation or thorough uncertainty propagation challenging using a costly simulation model alone. In this context, we propose an innovative multi-fidelity optimization under uncertainty algorithm with robust constraints that leverages inexpensive, low-fidelity simulations to alleviate computational burdens.

We employ a sample average approximation technique to transform the traditionally stochastic optimization problem into a deterministic framework. Our strategy involves integrating high-fidelity samples with a more extensive set of cost-effective low-fidelity samples for precise estimation of both the objective function and constraints. Specifically focusing on general convex optimization problems, we study the impact of multi-fidelity constraints on the robust optimization results. The incorporation of low-fidelity models may introduce bias into the constraint estimate, impacting optimization results while concurrently aiming to diminish the variance of the robust constraint estimate. This study conducts a comprehensive analysis of the trade-offs associated with multi-fidelity optimization, providing insights into how errors in low-fidelity sampling propagate through the optimization problem.

Additionally, we present preliminary results on a trajectory optimization under uncertainty problem, demonstrating safe and robust trajectory generation. We test a simple bi-fidelity strategy for accelerating trajectory optimization under uncertainty in the presence of robust constraints. Specifically, we accelerate the optimization using additional samples of low-fidelity models for assessing whether or not a risk constraint is violated. The low-fidelity model's purpose is thus to reduce the uncertainty in the estimate of constraint violation, at the expense of introduction of bias. Our empirical test on a simulation of glider dynamics tasked with avoiding a region indicates an order-of-magnitude less failures using the bi-fidelity strategy.

Recent advances in high-order methods for computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTIRATE TIME-INTEGRATION BASED ON DYNAMIC ODE PARTITIONING THROUGH ADAPTIVELY REFINED MESHES FOR CONVECTION-DOMINATED FLOWS

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ABSTRACT

A classic problem in the simulation of instationary convection-dominated flows is the restriction of the maximum stable timestep due to the presence of locally refined grid cells in the computational domain. When integrated in time with explicit methods the maximum stable timestep is restricted to some form of CFL condition which causes unnecessary effort in the non-refined parts of the domain, thereby impairing the computational efficiency. This is a problem that has been addressed by many authors in the past by means of various approaches going under names such as local time-stepping, multirate, and multiscale time integration.

Recently, a new approach to this problem has been proposed by Vermiere et. al. [1, 2] which is based on the idea of employing different stabilized Runge-Kutta schemes for differently sized cells in the domain. In particular, the approach developed in [1, 2] requires no changes in the spatial discretization which makes them easily implemented in codes which employ a method of lines (MoL) approach. In the original works [1, 2] the authors applied the so-called Paired-Explicit Runge-Kutta (P-ERK) schemes successfully to static, non-uniform meshes for the simulation of the compressible Navier-Stokes equations.

In [3] we explored the possibility to apply the P-ERK schemes to dynamically partitioned systems arising from adaptive mesh refinement (AMR). We show that despite the additional overhead due to the dynamic re-assignment of flagging variables speedup for a set of hyperoblic and hyperbolic-parabolic testcases can be realized compared to a range of state of the art Runge-Kutta methods. In particular, we consider hydrodynamic instabilities such as Kelvin-Helmholtz and Rayleigh-Taylor besides the ideal magnetohydrodynamics (MHD) rotor and the Orszag-Tang vortex for the visco-resistive MHD equations. We implemented the P-ERK schemes with dynamic partitioning in the open-source, high-order discontinuous Galerkin code Trixi.jl written in Julia.

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V - TANGENT KERNELS

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ABSTRACT

Machine learning (ML) has been profitably leveraged across a wide variety of problems in recent years. Empirical observations across many disciplines show that ML models from suitable functional spaces are capable of adequately efficient learning across a wide variety of disciplines. In this work (first in a planned sequence of three), we build the foundations for a generic perspective on ML model optimization and generalization dynamics. Specifically, we prove that under variants of gradient descent, “well-initialized” models solve sufficiently well-posed problems at "a priori" or "in situ" determinable rates. Notably, these results are obtained for a wider class of problems, loss functions, and models than the standard mean squared error and large width regime that is the focus of conventional Neural Tangent Kernel (NTK) analysis. The v - Tangent Kernel (vTK), a functional analytic object reminiscent of the NTK, emerges naturally as a key object in our analysis and its properties function as the control for learning.

We exemplify the power of our proposed perspective by showing that it applies to diverse practical problems solved using real ML models, such as classification tasks, data/regression fitting, differential equations, shape observable analysis, etc. We end with a discussion of the numerical evidence, and the role νTKs may play in characterizing the search phase (focus of the planned future work) of ML optimization which leads to the “well-initialized” models that are the crux of this work.

SciML in the real world
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LEVERAGING UNCERTAINTY QUANTIFICATION IN DEEP GENERATIVE MODELS FOR MANUFACTURING PROCESS DISCOVERY

Tuba Dolar[1], Daniel Quispe[1], Jian Cao[1] and Wei Chen[1]*

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ABSTRACT

Deep generative models (DGMs) are commonly employed for capturing complex, high-dimensional probability distributions, and subsequently generate realistic synthetic samples. One prominent use of DGMs is manufacturing process discovery where novel processes are inversely designed to satisfy desired process characteristics. Variational autoencoders (VAEs) are among DGMs and their architecture contains an encoder for compressing the input into a low-dimensional latent space and a decoder for reconstructing the dataset. A drawback of VAEs is the information loss caused by the encoding and decoding process which can produce unrealistic samples that lack the consistency of the input dataset. Additionally, a VAE model is valuable for exploring areas of the latent space for which data was unavailable initially. However, unrealistic processes would be discovered unless reliability of the generated samples are quantified. Quantifying uncertainties of the generated processes is critical for assessing these problems as high uncertainties would signal such issues. We propose leveraging epistemic uncertainty of the VAE decoder while designing a myriad of new manufacturing processes with varying energy inputs, workpiece materials, processing times, surface qualities, and tolerances. We start by introducing a manufacturing process language that allows the interpretation of a multitude of processes by defining process characteristics shared across diverse processes. This language is used for the analysis of 55 processes; including welding, machining, sintering, additive manufacturing, etc.; then a VAE model is used for extracting the complex relationships between these processes. In the VAE architecture, we implement Monte Carlo dropout in the decoder while generating new processes by sampling from the latent space. The adaptation of uncertainty quantification allows obtaining probability distributions for the process characteristics of the generated process instead of point predictions. These probability distributions are valuable for evaluating how certain the model is in terms of satisfying the desired process characteristics. Contributions of our work include 1) identifying probability distributions for the desired process characteristics instead of point predictions in manufacturing process discovery, 2) allowing the user to validate the designed manufacturing process by assessing whether the process characteristic variations are within acceptable limits, and 3) driving further data collection efforts for enhancing the input database. Using the inverse design of a process that uses mechanical and thermal energy, we demonstrate the benefits of our approach in three process discovery cases. Firstly, we search for processes that achieve high removal speeds, then tight tolerances in forming processes, and finally large volume prints in additive manufacturing.

16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics

July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FORMULATIONS OF GRIFFITH PHASE-FIELD FRACTURE WITH STRENGTH: ON MODEL VALIDATION AND VARIATIONAL THEORIES

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ABSTRACT

We discuss several recent advances in phase-field models of fracture that illustrate the importance of accurately representing material strength. Our motivation stems from a recent study on model validation, consisting of simulations of crack nucleation from V-notches in quasi-brittle metallic alloys. The study illustrates how model validation based on an energetic threshold for nucleation simply fails to reproduce the results across the full spectrum of V-notches. Instead, our analysis indicates that a stress envelope is capable of adequately explaining nucleation, and that any complete theory of phase-field fracture must account for arbitrary material strength. We will discuss the merits of such a complete theory, as demonstrated by its ability to resolve long-standing misconceptions behind the Brazilian test. Additional results from problems in dynamic, brittle fracture will also be presented to support the necessity of such a complete theory. Finally, I will share a recent result that illustrates how an existing phase-field model of fracture with arbitrary material strength can in fact be recast as a variational theory.

Scientific machine learning for geophysical applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPLAINABLE ARTIFICIAL INTELLIGENCE FOR WEATHER EXTREMES

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ABSTRACT

Extreme weather events can potentially pose threats to human lives and cause significant economic losses. Predicting such events and implementing appropriate responses can mitigate their harmful impacts. In this work, we propose a new explainable AI framework to predict and better understand extreme events, based on [1]. By pinpointing the relevant information used by neural networks, we can bridge AI knowledge to existing physical knowledge. As part of this work, we also provide a benchmark dataset of extreme events that researchers can use to test their AI solutions within this context.

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Multi-scale and machine learning-based modeling methods for optimization and design of composites
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A DAMAGE PHYSICS-GUIDED APPROACH TO ACOUSTIC EMISSION SIGNALS IDENTIFICATION IN COMPOSITE MATERIALS

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ABSTRACT

Cluster techniques have proven to be highly effective in identifying acoustic emission (AE) signals of composite damages. Nevertheless, traditional clustering models usually ignore the underlying physical mechanisms of the complex failure process of composites, limiting the comprehensive understanding and analysis of damage mechanisms. Notably, throughout all stages of damage evolution in the composite laminates under load, except for the initial stage that is dominated by matrix cracking, all the subsequent stages are characterized by the combination and interaction of multiple damage modes. Therefore, this study proposes an AE signal identification method guided by the physical mechanisms of damages in composite materials. Firstly, a sliding window is utilized to capture short-term variations of the AE energy within the window over a time series. Aligning with the initiation and accumulation process of micro-damages observed during penetrant detecting, the AE data are segmented to distinguish the time periods in which damage modes such as matrix cracking, crack coupling-interfacial debonding, delamination, and fiber breakage occur and develop. Secondly, given that the AE data in the first stage is related solely to matrix damage, a classification model of the semi-supervision guided deep neural network is established to predict matrix damage in the second stage. A confidence threshold is then set and a clustering algorithm is applied to the second stage data that was not explicitly labelled by the proposed classification model. The classification model is used to identify known damage mode, while clustering algorithm is used to explore and define new damage modes. The results of the classification and clustering are then combined for labelling, and the classification model is further optimized and updated by the alternative use of classification and clustering. The results of the classification and clustering will then be used as the input of the next stage. The above process is repeated, during which the cross-stage learning capability of the classification model is enhanced iteratively, as such to finalize a deep neural network classification model. Finally, the full AE data labels are updated to provide comprehensive damage identification. Our approach incorporates domain knowledge and provide new perspectives and more explanatory solutions for damage identification in composites.

Emerging frontiers and methods in digital manufacturing: Modeling, simulation, and beyond
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DESIGN OF IN-MOLD DECORATION MOLD FOR COMPLEX THIN-WALLED PARTS

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ABSTRACT

In order to address the issues of warping deformation and long-term production of complex thin-walled parts during In-Mold Decoration (IMD) production, the structure design of the IMD mold was carried out with the upper cover of the refrigerator humidifier as the production object. To ensure the flow characteristics of molten plastic in the mold during the injection molding process, the hot-runner mold is improved to mix cold-and-hot-runner, that is, the main-runner is set as a hot-runner, the sub-runner is set as a cold-runner, and use a multi-point injection cold gate solution. And construct a complex structure numbering method to arrange and design various complex core pulling and parting mechanisms, design a special structure with a slanted top to simultaneously pull cores from two inverted buckles in the same direction. Simultaneously complete the molding, parting, and demolding and ejection of plastic parts using a tilting mechanism. Finally, design the cooling system and demolding mechanism separately. To optimize product quality and improve production efficiency, providing theoretical and empirical support for the production of complex thin-walled parts with in mold injection molds. Based on Moldflow software, the final flow of plastic part warping deformation is analyzed. The maximum warping deformation of the designed product is 0.7055mm, while the maximum warping deformation of the traditional cold runner mold is 0.8519mm, reducing the warping deformation of the product.

Machine learning for design tasks and inverse problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RANDOMIZED NEURAL NETWORKS FOR COMPUTING INVERSE PARAMETRIC PDE PROBLEMS

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ABSTRACT

We present a method for computing the inverse parameters and the solution field to inverse parametric partial differential equations (PDE) based on randomized neural networks. This extends the local extreme learning machine technique originally developed for forward PDEs to inverse problems. We develop three algorithms for training the neural network to solve the inverse PDE problem. The first algorithm (termed NLLSQ) determines the inverse parameters and the trainable network parameters all together by the nonlinear least squares method with perturbations (NLLSQ-perturb). The second algorithm (termed VarPro-F1) eliminates the inverse parameters from the overall problem by variable projection to attain a reduced problem about the trainable network parameters only. It solves the reduced problem first by the NLLSQ-perturb algorithm for the trainable network parameters, and then computes the inverse parameters by the linear least squares method. The third algorithm (termed VarPro-F2) eliminates the trainable network parameters from the overall problem by variable projection to attain a reduced problem about the inverse parameters only. It solves the reduced problem for the inverse parameters first, and then computes the trainable network parameters afterwards. VarPro-F1 and VarPro-F2 are reciprocal to each other in some sense. The presented method produces accurate results for inverse PDE problems. For noise-free data, the errors of the inverse parameters and the solution field decrease exponentially as the number of collocation points or the number of trainable network parameters increases, and can reach a level close to the machine accuracy. For noisy data, the accuracy degrades compared with the case of noise-free data, but the method remains quite accurate. Several numerical examples will be presented to demonstrate the characteristics and accuracy of the current method. It will be compared with the state-of-the-art neural network-based method for inverse PDEs.

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Advanced computational modelling of wood, wood-based products, bio-composites, and timber structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELLING THE MECHANICAL BEHAVIOUR OF SANDWICH PANELS MADE OF ARUNDO DONAX CORE AND FLAX FIBRE REINFORCED EPOXY COMPOSITE SKINS

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ABSTRACT

In recent years, the use and interest in eco-friendly solutions in the field of civil engineering and construction have significantly increased. Specifically, building panels represent a key area where the use of bio-based materials offers significant opportunities to improve the sustainability of the life cycle of constructions [1].
This study aims to model the behavior of a sandwich panel with a core made of Arundo Donax rings and skins made of flax fiber-reinforced epoxy composites. The rings and skins are connected using an epoxy resin, which, during the curing phase, fills the voids inside the core, ensuring a connection between the rings constituting the core itself. A finite element model has been developed to simulate the nonlinear behavior of the panel subjected to bending tests, using Abaqus software.
It is assumed that the non-linearity of the panel is due to the bonding area between the skins and Arundo rings. Arundo rings and the skin have been modeled as orthotropic materials. The model includes cohesive surface contacts between the skins and bamboo rings, for which a damage initiation stress value was imposed, derived from pull-off experimental tests. The contact between elements of the Arundo core is modeled using hard contact in the normal direction and a penalty to consider friction in the tangential direction.
The model has been validated with the experimental campaign described in [2]. Subsequently, the model was used to conduct a parametric analysis to understand how the performance is influenced by geometric parameters such as ring diameters. During the parametric study, it was observed that with an increase in the diameter of Arundo rings in the core, there was an increase in the maximum load and the maximum failure stress of the panel, panel bending stifness, while the contact area between the rings in the core and the skins remained constant.

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RAY TRACING FOR INVERSE DESIGN OF GRADED METAMATERIAL WAVEGUIDES

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ABSTRACT

While periodic metamaterials have been well studied for guiding elastic waves, spatially graded metamaterials offer a much larger but comparatively unexplored design space. Due to the bottleneck of modeling efficiency, the use of spatial grading for wave control has been limited to simple gradings or long wavelengths. In this work, we present an inverse design methodology that leverages ray tracing as an efficient forward modeling tool. An optimization framework is developed to minimize cost functions based on ray trajectories [1]. In this framework, efficient forward modeling is provided by ray tracing, while the adjoint state method is used to obtain cost function gradients for gradient-based optimization. This provides a flexible and efficient methodology for designing arbitrary spatial gradings to control dispersive high-frequency wave propagation. We demonstrate the design of graded mass-spring networks as well as graded truss metamaterials modeled with beam finite elements. Example design objectives include elastic wave focusing, broadband wave steering, and frequency sorting. These objectives are out of reach of periodic architectures, demonstrating the potential of spatially graded metamaterials for wave guidance applications.

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Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXTENDED B-SPLINE MATERIAL POINT METHOD FOR STRONGLY COUPLED DIFFUSION IN HYDROGELS

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ABSTRACT

The Material Point Method (MPM), a hybrid Eulerian-Lagrangian particle-based continuum approach, emerges as a robust alternative to conventional mesh-based finite element methods. Its effectiveness in handling extreme deformations and no-slip contact conditions without requiring additional algorithmic treatments makes it particularly promising. When modeling highly deformable materials like elastomers, hydrogels, and biological tissues, an implicit time integration is preferred due to its computational robustness for modeling and testing materials under quasi-static conditions. However, challenges arise, particularly within implicit solvers, including the ill-conditioning of the stiffness matrix due to fewer material points near the boundaries and the complexities involved in imposing boundary conditions. Furthermore, modeling at the quasi-compressible limit of soft polymeric materials requires multi-field discretizations, such as the displacement-chemical potential, to capture strongly coupled diffusion in hydrogels. Mixed discretizations, if not handled correctly, may lead to numerical instabilities related to the so-called inf-sup condition. In this presentation, we will address these challenges using a subdivision-stabilized mixed formulation and further extend the subdivision-stabilization to the extended B-spline technique. Additionally, we will exploit the Nitsche method for imposing boundary conditions. Through the use of the Nitsche method, essential boundary conditions are weakly imposed directly on the Lagrangian particles instead of the Eulerian background grid where the solution is obtained. The extended B-spline shape functions address the ill-conditioning by interpolating the displacement and chemical potential fields near the detected physical boundaries to the interior ones using polynomials. The developed subdivision-based extended B-spline method achieves an oscillation-free, inf-sup stable mixed discretization when modeling hydrogels under instantaneous loading. We will test the stability and accuracy of our mixed B-spline MPM at extreme deformations and verify it by comparing our results with benchmark problems, including the buckling of cylindrical hydrogels, confined-compression of hydrogel beads, and swelling deformations under constraints. These examples showcase the effectiveness of the developed particle-based method in modeling practical soft material applications without encountering any numerical instabilities.

Machine learning for design tasks and inverse problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STRUCTURAL OPTIMIZATION THROUGH GENERATIVE ADVERSARIAL NETWORKS

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ABSTRACT

The finite element method (FEM) is a well-known approach to solve partial differential equations. It has important applications in structural engineering. A notable example is topology optimization (TO), in which the distribution of material in a structure is altered to optimize a goal, such as weight minimization and structural natural frequency maximization. TO involves, at each iteration, the solution of a structural problem via FEM, which could lead to high computational costs. Therefore, a line of research developed over the years focusing on using machine learning (ML) to accelerate TO. Particularly, researchers proposed Artificial Neural Networks (ANNs) to significantly speed-up the process by eliminating the iterative algorithm which is intrinsic to TO. Since ANN is a supervised ML method, in the present work, first a dataset of 138,600 2D finite element analysis (FEA) cases is generated, containing FEA inputs (boundary conditions), volume fraction, strain energy density and von Mises fields, and final topologies. Afterwards, following the standard pipeline for ML projects, the dataset is filtered. Many samples, with diverse types of problems, are removed from the dataset. This increases the quality of the data, avoiding samples which could mislead or slow down model training. The issues considered are: plasticity, intermediary densities, geometrical nonlinearities, disconnections, and isolated features. In total, 12% of the initially generated samples were filtered out. With the data filtered, the model is trained to map fields of physical quantities, such as the von Mises stress, to the final optimized structure. Over the years, distinct types of generative deep learning approaches were applied to TO, such as variational autoencoder and generative adversarial networks (GANs), which is composed of two ANNs, the generator and the discriminator. The present work uses a specific development of this framework, Wasserstein GANs (WGANs). Additionally, the generator is inspired by a recently proposed architecture (“ConvNeXt”); and the loss function used to train this network was also influenced by the “pix2pix” approach. The designs obtained by the approach developed adhere better to TO solutions, when compared to recent results in the field. Furthermore, these improvements are achieved with much less computational cost than both the standard TO method and an alternative GANs model. Finally, interpretability (XAI) techniques were also applied to the trained networks, to better understand what information in the input is more relevant, and how the output was determined.

Advance modeling and simulation in complex porous media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BUBBLE-STABILISED POLYTOPAL SCHEME FOR FLOWS IN FRACTURED MEDIA WITH FRICTIONAL CONTACT

Jerome Droniou[*1], Guillaume Enchéry[2], Isabelle Faille[2], Ali Haidar[3] and Roland Masson[3]*

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ABSTRACT

We present a numerical scheme, applicable on generic polytopal meshes, for a model of flows in porous medium with fractures. The model is mixed-dimensional, that is the rock matrix is represented as a 3D model in which fractures are 2D hypersurfaces, that takes into account poro-mechanical effects. We consider frictional contact, taking into account the Coulomb law via Lagrange multipliers. We use a hybrid finite volume scheme for the flow, a piecewise constant space for Lagrange multipliers, and a low-order fully discrete scheme for the matrix displacement; this scheme uses vertex unknowns complemented by "bubble"-like degree of freedom, designed to ensure the inf-sup condition of the displacement jumps with the space of Lagrange multipliers. This fully discrete scheme is equivalent to a Virtual Element scheme. We prove the inf-sup condition, as well as the convergence of the scheme in the case of pure contact mechanics. Numerical tests for the complete coupled problem will also be presented.

Methods for identification, machine learning, and uncertainty quantification of reduced order models of coupled systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADVANCING UNDERSTANDING OF HIGH-DIMENSIONAL QUASI GEOSTROPHIC SYSTEMS.

Ahmad Droobi[*1] and Mustafa Mohamad*[1]

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ABSTRACT

The goal of this work is to advance our understanding of high-dimensional Quasi Geostrophic (QG) systems through partial measurements in the context of time-sequential state estimation. Our focus lies in the accurate reconstruction of the turbulent QG flow field's Eulerian energy spectra, from a stream of noisy measurements derived from Lagrangian tracers or drifters. These tracers, instrumental in atmospheric and oceanic measurements, serve as dynamic data collectors, offering real-time insights as they traverse the velocity field.

Employing numerical simulations, we solve the QG equation to obtain the true values of the high-dimensional QG system. Subsequently, we seek to design an innovative hybrid filter, incorporating ensemble Kalman filter and particle filter methodologies. This filter aims to predict the recovery and behavior of the QG system, matching predictions as closely as possible with the ground truth derived from numerical simulations.

This work extends conditionally Gaussian nonlinear filters that are tailored for Lagrangian data assimilation. We address questions concerning the extent to which turbulent Eulerian energy spectra can be recovered through assimilation of Lagrangian trajectory data. We quantify the recovery of various energetic scales relative to the ground truth and assess the impact of model error through reduced order models.

Demonstrating the efficacy of our hybrid filter, we showcase high recovery skill in reconstructing the two-dimensional turbulent energy spectra. The proficiency is shown across diverse scenarios, including an inverse cascade spectrum with a slope of \begin{math}k^{-5/3}\end{math} and a direct cascade spectrum with a slope of k^{-3}. Our approach involves localization of the covariance matrix, rendering it more computationally efficient compared to exact filters. We assess spectral energy recovery skill on the number of tracers and the spectral truncation grid size. The overall goal is to contribute to the development of a filter that can recover the behavior of the QG system from partial Lagrangian measurements.

Numerical modelling of composite materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

OPTIMAL DESIGN OF GRAPHENE-REINFORCED COMPOSITES USING SHUNTED PIEZOELECTRIC SYSTEMS FOR OPTIMAL VIBRATION ATTENUATION

Maria-Styliani Daraki[1], Georgios Drosopoulos[2], Georgia A. Foutsitzi[3] and Georgios Stavroulakis[1]*

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ABSTRACT

Smart structures exploit the synergy between several coupled physical phenomena to produce materials and structures with enhanced properties. Such structures incorporate integrated sensors and actuators, mechanical and electronic components and control. The design of smart structures is a multidisciplinary challenge, which is of high importance for viability and resilience of industry. Usage of piezocomposites with integrated nonlinear shunted circuits for vibration suppression improves effectiveness and accuracy of many high-value products. The finite element method is widely used to simulate the mechanical response of composite materials and multi-physics problems [1], [2]. In this work a numerical investigation is conducted on small scale beams aiming to improve their vibration response by applying piezoelectric shunted circuits. Finite element models are developed in MATLAB, simulating graphene-reinforced nanocomposite piezoelectric beams with shunted circuits under vibration excitations. Piezoelectric materials are applied to the beams to allow for the interaction between electric charge and mechanical deformation. In addition, shunted circuits, which are paired with piezoelectric elements, are used to provide damping (vibration suppression) of one or more critical eigenfrequencies [3].
To derive the optimal vibration response, a particle swarm optimization (PSO) algorithm is adopted. Optimization is then aimed to minimize the vibration amplitude as well as optimize the mechanical and electrical parameters of the investigated system. Results illustrate the accuracy and reliability of the present finite element formulation for the considered frequency response analysis of the piezoelectric composite beams.

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Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL INVESTIGATION OF NON-NEWTONIAN FLUIDS IN SINGLE SCREW EXTRUDERS: HEAT TRANSFER AND CFD MULTIPHYSICS STUDIES

Pablo Druetta[*1], Tim Kousemaker[1] and Francesco Picchioni[1]*

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ABSTRACT

Plastic extrusion is one of the cornerstones of the polymer processing industry and it plays a pivotal role in manufacturing a vast myriad of products, for instance pipes, films and profiles, and it is also used in the automotive industry and consumer goods. Since its first application, it has completely change the way we create plastic components, becoming in an essential tool in many industry sectors. Therefore, in order to achieve an efficient, cost-effective, and sustainable production, the completely understanding of the process is considered vital to minimize its environmental impact. Moreover, in recent years, Computational Fluid Dynamics (CFD) has revolutionized our ability to analyze and optimize, among others, plastic extrusion processes. CFD offers a powerful tool to simulate, design, optimize and predict the behavior of the intricate fluid dynamics and thermal phenomena that govern plastic material behavior within the barrel. This allows gaining insight into the complex interplay of factors that impact extrusion performance, such as temperature distribution, pressure gradients, melt flow behavior, screw geometry, and material properties. We present the study of a 3D single screw extruder model. The definition of the physical and mathematical model is introduced in detail and a series of steady-state studies analyzing the behavior of the system are discussed. In order to develop a suitable model, mass, momentum and heat conservation equations are modelled, coupled with non-Newtonian fluid models in a novel approach, where a shear-thinning/-thickening, temperature-depending rheology correlation is modelled in COMSOL, in order to reproduce the processing of polymer solutions. Steady-state studies show that considering only shear-thinning behavior underestimates crucial parameters such as pressure, viscosity and thermal profile due to differences in the velocity field and viscous stress tensor. Moreover, the influence of the screw in the heat transfer process cannot be considered negligible, since the metal creates a recirculation circuit, which influences the polymer entering into the barrel. These studies provide the first step in a series of further advances in 3D modelling of extrusion processes, by considering the multiphysics behavior in a dynamic, rotating, polymer processing machinery.

Advances in damage & fracture modeling of multiphysics materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FAILURE SIMULATION OF BRITTLE MATERIALS UNDER DYNAMIC LOADS BASED ON SCALED BOUNDARY FINITE ELEMENT METHOD

Chengbin Du[*1] and Zhiwei Zhao*[1]

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ABSTRACT

In this study, a nonlocal multiscale damage model [1] that considers the effect of a strain rate for quasi-brittle materials is presented. The scaling centre of each scaled boundary finite element method (SBFEM) subdomain was selected as the material point, and the bond connecting two material points was referred to as the material bond. Microscopic damage was quantified based on the stretch rate of the material bond, and macroscale topological damage was calculated by taking the weighted average of the microscopic damage over the bonds within the influence domain. The bell distribution function is chosen as the weight function in the calculation of the nonlocal weight function. To account for the impact of the strain rate during dynamic loading, an effective rate R [2] is introduced to enhance multiscale damage by modifying the damage threshold and bond softening coefficient throughout the analysis process. By analysing the energetic degradation function of the phase field, which establishes a connection between the macroscale topological damage and energy-based damage, a nonlocal multiscale damage model was incorporated into the framework of the SBFEM. Four typical dynamic cracking examples were simulated using the proposed model, and the results were compared with the relevant experimental results and references. The results show that the method is suitable for accurate dynamic failure simulation in quasi-brittle materials. Moreover, the results indicate that the proposed method can spontaneously simulate dynamic crack bifurcation without introducing additional crack bifurcation criteria. For a compact tensile test of concrete under different loading rates, the method proposed in this study can accurately simulate the corresponding failure modes. The results also show that without considering the effect of the strain rate, the damage develops rapidly in an unconstrained state, which is inconsistent with the actual case.

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PROGRAMMING PATCHY PARTICLES FOR MATERIALS ASSEMBLY DESIGN

Chrisy Xiyu Du[1], Ella King[2], Qian-Ze Zhu[3], Samuel Schoenholz[4] and Michael Brenner[3]*

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ABSTRACT

Soft Materials are ubiquitous in everyday life and are crucial in many different forms of revolutionary technologies. One property of Soft Materials is their ability to self-assemble into intricate structures from a finite set of building blocks with continuously tunable parameters. This giant design space of building blocks is a double-edged sword: on one side it provides researchers infinite possibilities to design building blocks for targeted functions, while on the other side it might take forever to search the design space. Here, we propose a new inverse design method that captures both interaction and geometry of building blocks. By enabling rigid body functionalities in JAX-MD, an end-to-end differentiable molecular dynamics engine, we can create soft materials model with components that are simple enough to design yet powerful enough to capture complex materials properties. In this talk, I will discuss the implementation of the methods alongside examples to showcase its potential applications.

AUTOMATED MULTILEVEL SUBSTRUCTURING BASED ON LDLT FACTORIZATION

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ABSTRACT

Generalized eigenvalue problems are crucial in finite element modal analysis, yet traditional methods typically struggle with efficient resolution of a large number of vibration modes. Kaplan's classic implementation of automated multilevel substructuring (AMLS)[1] significantly advanced the efficiency of solving numerous modes in FEA. This paper presents new and improved AMLS implementations designed for large scale eigenvalue problems, such as those involving 30 million DOFs.

In our research, it was found that the block Gaussian elimination of stiffness matrices in the classic AMLS can effectively be replaced by widely-adopted LDLT factorizations in FEA. The key to our implementations, explicit automated multilevel substructuring based on LDLT factorization (LDLT-EAMLS) and implicit automated multilevel substructuring based on LDLT factorization (LDLT-IAMLS), is built upon the existing and highly-optimized LDLT factorization used in applications and enables the bypassing of the LDLT process. The computational cost of LDLT-EAMLS including factorization is equivalent to that of the classic AMLS. As the size of the problem increases, the cost of LDLT factorization may escalate, making the advantages of LDLT-EAMLS even more pronounced. In addition, LDLT-EAMLS significantly reduces the storage requirements in comparison with the classic AMLS.

For problems involving more than ten million DOFs, both the classic AMLS and LDLT-EAMLS approach impracticality. This is primarily due to the exorbitant cost associated with the explicit computation of diagonal blocks in the condensed mass matrix, as size of the substructures, particularly the interface substructures, expands. These methods become increasingly challenging with the escalation in the size of the substructures. To address this challenge, LDLT-IAMLS was developed. The algorithm solely performs the operations of mass matrix-vector multiplication without explicitly forming the block mass matrix. Compared to explicit methods, LDLT-IAMLS noticeably reduces the need for solving linear equations, offering substantial benefits for large-scale problems.

Numerical tests with 1 million DOFs demonstrate that LDLT-EAMLS reduces solution time by approximately 30% to 50% compared to the classic AMLS. Furthermore, in larger-scale problems, such as those involving 7 million DOFs, LDLT-IAMLS exhibits an acceleration of over 3 times compared to LDLT-EAMLS. Additionally, it has been successfully demonstrated that LDLT-IAMLS can efficiently solve problems with up to 32 million DOFs.

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Uncertainty quantification and reliability analysis in engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FREE VIBRATION ANALYSIS OF AXIAL-LOADED BEAMS WITH VARIABLE CROSS SECTIONS AND MULTIPLE CONCENTRATED ELEMENTS

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ABSTRACT

A transfer matrix method is used to study free vibration characteristics of an axial-loaded Euler–Bernoulli beam with variable cross sections and multiple concentrated elements in the article. The differential equation for bending vibrations of the beam element is solved by the Frobenius method, and the solution is in power series form. Then, the transfer matrix method is applied to establish the state vector equation for both ends of the beam. Combined with boundary conditions, the frequency equation is obtained and expressed in a two-order determinant. The numerical results in this article are compared with those of the finite element method, which illustrates the accuracy of the method we proposed. The influence of the size of each concentrated elements and axial force on the natural frequency coefficients and the influence of the concentrated elements on the first critical buckling load are discussed.

Multiphysics biomechanics of bio- and bio-inspired soft materials: Theory, simulation and experiments
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MECHANICS MODEL AND INJURY MECHANISM OF BLAST-INDUCED TRAUMATIC BRAIN INJURY

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ABSTRACT

In the context of modern warfare, Traumatic Brain Injury (TBI), particularly blast-induced Traumatic Brain Injury (bTBI), has seen a marked increase, becoming a hallmark injury. This research domain is inherently interdisciplinary, encompassing mechanics, medicine, and biology, and is challenged by unclear injury mechanisms and a lack of evaluative indicators and methods. This paper establishes a mechanics model to elucidate the mechanical injury mechanism of bTBI, with significant findings including:

Development of a micromechanical constitutive model of brain tissue, integrating diffusion tensor imaging data. This model considers the deformation and damage of anisotropic axons and isotropic matrix, alongside an axonal equivalent strain-based damage initiation criterion. This enhances understanding of brain tissue's nonlinear behavior, anisotropic response, strain rate dependency, and specific damage behavior under complex stress states.

Creation of a high-precision fluid-structure coupling numerical model elucidating the mechanical mechanisms of bTBI from blast overpressure transmission and skull deformation. We determined that the direct transmission of the blast wave forms the positive peak of Intracranial Pressure (ICP), while skull deformation leads to the negative peak and oscillatory ICP pattern. The skull-brain tissue interface emerges as a critical vulnerability zone in blast wave propagation.

Construction of a multi-layer head structure model reflecting angular acceleration response characteristics, and proposing a bTBI indicator based on axonal strain rate. Under acceleration loading, the corpus callosum and upper brainstem exhibit high-speed axonal deformation responses, correlating with medically identified injury areas. This suggests that excessive axonal strain rate is a primary cause of diffuse axonal injury under acceleration overload.

Development of a dynamic test system using a high-fidelity surrogate head and neck model. We established an evaluation method for bTBI based on a shock tube experimental platform, proposing a comprehensive standard incorporating ICP and acceleration indicators. The fluid-structure coupling simulation under shock tube conditions confirms the platform's accuracy in measuring physical responses during blast overpressure propagation.

These results offer a theoretical foundation for medical diagnosis and protection strategies in bTBI, presenting substantial scientific significance and engineering application value.

LAGRANGIAN PARTICLE METHOD FOR MULTI-PHASE AND MULTI-PHYSICS PROBLEMS: A HIGH-PRECISION AND VERSATILE APPROACH

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ABSTRACT

With the recent breakthrough advancements, the high-precision particle method has gradually become a reliable and mature method, overcoming the fundamental limitations in accuracy, stability, and boundary condition within traditional particle methods. This presentation provides an overview of its latest advancements and applications in multi-phase and multi-physics problems.

First, high-precision schemes are typically derived from the least squares method and Taylor series expansion. In this process, various boundary conditions have been newly considered as additional constraints for straightforward and precise imposition. Second, the biased neighbor support is found to be the main reason for error accumulation and numerical instability [1]. Two strategies have been combined to avoid biased neighbor support and instability: particle shifting techniques and accurate free-surface detection. Various particle shifting techniques were proposed for internal and boundary-vicinity particles to regulate particle distributions. Novel free-surface-detection conditions based on the employed high-precision schemes have been developed to effectively maintain the stability near free surfaces [1]. Third, the high-precision particle method provides new promise for multiphase flows with high-density ratio by separately calculating the gas and liquid phases. In this approach, the free-surface-tension model was a key bottleneck. Fortunately, high-precision particle method can straightforwardly realize an accurate and versatile model for the free surface tension [2]. An exact sharp-interface model can then be proposed for bubble flows, even surpassing conventional mesh methods in capturing interface coalescence and breakup. Finally, the conventional phase-change models and fluid-solid interaction models can be easily integrated into the high-precision particle method, enabling the reliable simulations of multi-physics problems.

Before multi-physics applications, the developed high-precision particle method has been verified and validated through various theoretical and experimental benchmark cases without tuning parameters. Meanwhile, the developed particle method can consistently produce reliable smooth velocity and pressure distributions. Lastly, various applications in nuclear severe accidents and metal additive manufacturing demonstrated promising capabilities of the developed method.

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Acknowledgement

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Advances in multi-scale, multi-material, and multi-component Topology Optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTI-SCALE VARIABLE STIFFNESS DESIGN OPTIMIZATION OF COMPOSITE LAMINATES FOR MINIMUM STRUCTURAL COMPLIANCE WITH CONSIDER ADDITIVE MANUFACTURING FIBER CONTINUITY

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ABSTRACT

Structural lightweight design is the eternal theme of aerospace equipment structure. Fiber-reinforced composite laminates have become the ideal material and structural form for lightweight and functionalization aerospace structures due to their excellent material properties and the designability of their material microstructures. Especially in recent years, with the rapid development of continuous fiber additive manufacturing technology, which provides the possibility to manufacture optimized multi-scale fiber-reinforced composites. One of the challenges in the variable stiffness design optimization of discrete fiber composite laminates is how to avoid the explosion of design variable combinations caused by the increase in the number of alternative discrete fiber laying angles. The Normal Distribution Fiber Optimization (NDFO) interpolation scheme has the numerical advantage that the design variables do not increase with the increase in the number of alternative discrete fiber laying angles. However, the traditional NDFO interpolation scheme uses the normalization penalty parameters, which leads to the discrete fiber laying angle selection falling into the local optimal prematurely. At the same time, the normalization of penalty parameters ignores the convergence differences of discrete fiber laying angles at different element in the macro-scale structure topology, leading to time-consuming and unstable optimization iteration. Therefore, considering the difficulties and challenges in the multi-scale variable stiffness design optimization of fiber-reinforced composites, an improved Adaptive Normal Distribution Fiber Optimization (ANDFO) interpolation scheme is proposed, and the feedback mechanism of the convergence rate of the element design variable and the objective function is introduced to realize the adaptive reduction of the penalty parameters. Based on the modified ANDFO interpolation scheme, a multi-scale optimization model of fiber-reinforced composite laminates is established considering the macro-scale structure topology and micro-scale discrete fiber laying angel selection. The explicit sensitivity of the objective function of minimizing structural compliance to the macro-scale topological design variables and the micro-scale fiber laying angle design variables is derived. Considering the manufacturability of additive manufacturing based on the optimized design results, a multi-scale nonlinear continuous filtration strategy for discrete fiber laying angle is adopted to improve the continuity of local fiber laying path. Numerical examples systematically compare the differences between the proposed ANDFO and the traditional NDFO model in fiber laying path and objective function, verifying the effectiveness of the proposed interpolation scheme.

Current trends and advances in enriched finite element methods and coupled simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NON-INTRUSIVE MULTISCALE STRUCTURAL MODELING WITH STANDARD AND GENERALIZED FINITE ELEMENT METHODS

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ABSTRACT

High-fidelity resolution of fine-scale defects, such as cracks and localized material damage, and structural features, such as welds and bolted connections, is critical for the accurate prediction of service life or failure of structures. Three-dimensional models with detailed meshes and advanced modeling techniques are usually required to capture accurate fine-scale responses. However, adopting such models on the structural/global scale is computationally inefficient and sometimes impractical for problems involving a large number of local features. A coarse mesh is often sufficient for predicting the global behavior of a structure.

In this talk, we present a multiscale computational framework that couples Abaqus models and 3D Generalized FEM discretizations based on numerically-defined enrichment functions – the so-called GFEMgl. The structural-scale problem is modeled in Abaqus using a coarse mesh of 3D or shell elements suitable for capturing the macro-scale response of the structure. Fine-scale problems solved in parallel provide enrichment functions for the GFEMgl. These functions enable the GFEMgl to accurately approximate localized phenomena such as crack propagation and material damage using coarse meshes. The interactions between structural (Abaqus) and GFEMgl models are captured using the Iterative Global-Local (IGL) method. Numerical examples show that this methodology provides accurate solutions even when a classical global-local/sub-modeling analysis fails.

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Geometric mechanics formulations and structure-preserving discretizations for continuum mechanics and kinetic models

July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ENERGY PRESERVATION OF HIGH-ORDER MIMETIC DIFFERENCES FOR SYSTEMS OF CONSERVATION LAWS

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ABSTRACT

We prove energy conservation of high-order mimetic difference schemes for linear and nonlinear systems of conservation laws. Furthermore, we numerically validate the theoretical foundation of our approach by showing that high-order mimetic schemes converge to the exact solution of general nonlinear systems of conservation laws preserving all quantities of interest.

AN INVERSE-FREE KRYLOV ALGORITHM FOR COMPUTING THE FIRST EIGENPAIRS OF NONLINEAR SYMMETRIC EIGENVALUE PROBLEMS

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ABSTRACT

We propose an algorithm to compute the set of eigenpairs corresponding to a given number of smallest eigenvalues of a nonlinear, positive definite eigenvalue problem. This has application not only to assess the vibration response of a structure but also to model its general dynamic behavior in terms of an advanced modal analysis, which has been previously developed. The method generalizes an inverse-free Krylov subspace algorithm, which now can solve nonlinear eigenvalue problems expressed either exactly, in terms of closed-form functions, or as a matrix power series. Once an eigenpair is obtained, we resort to a general deflation scheme that may be considered a penalty function accrued to the original problem to prevent already obtained results from being re-evaluated. The proposed algorithm works even when the introduced penalty function does not reflect the problem's symmetry, which is also assessed numerically. When the combined subspace iteration and the deflation schemes are applied to an eigenvalue problem in terms of closed-form, exact analytical matrix functions, we may also consider viscous damping, which is associated with a complex symmetric problem. Convergence is assessed for a few numerical examples. We show that classical preconditioners may be applied to save computational time when dealing with large linear algebra problems, as also illustrated.

New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION METHOD APPLIED TO FLUID FLOW CONSIDERING RESONANCE FREQUENCY CONSTRAINT

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ABSTRACT

Greenhouse gases (GHG), such as carbon dioxide (CO2), have detrimental effects on the environment. Consequently, nations worldwide are developing projects to mitigate these effects, such as carbon capture and storage (CCS). These projects typically involve three stages: separation of CO2 from other gases, compression and transportation, and injection. The compression stage involves increasing pressure and temperature beyond the critical point. Due to these conditions and the high rotation velocities, in the compressor impeller's design, it is necessary to consider compressible flow and take care of resonance frequency. This work approaches some of these considerations: compressibility and maximization of resonance frequency. The Topology Optimization Method (TOM) is used due to its capability to achieve non-intuitive topologies and initiate the optimization process from an arbitrary initial guess. A weighted multi-objective function is defined considering the minimization of flows viscous dissipation and maximization of the solid material resonance frequency. A volume constraint is also considered. The FEniCS finite element software is used to solve the state equations, considering the perfect gas model, and the pyadjoint library is used to compute the fluid flow sensitivities by automatic differentiation in conjunction with a matlab routine to calculate the resonance frequency sensitivity. The SciPy optimization library is used to update the design variables. The results show channel designs with optimized energy dissipation and improved resonance frequency.

Recent advances in numerical methods for interface problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MIXED FINITE ELEMENT APPROACH TO SOLVING LINEAR COSSERAT EQUATIONS

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ABSTRACT

The objective of this study is to explore the equations that govern Cosserat materials in three spatial dimensions [1, 2], also known in the engineering community as (micro-)polar materials [3]. A Cosserat material extends linearized elasticity equations by adding local rotations as independent variables as well as displacements, providing greater generality for modeling complex materials, such as granular media, cell-like and crystallized solids, and composite porous media [4]. Previous studies have focused on finite element methods for the second-order formulation, particularly in terms of displacement and rotation [5,6], but our interest lies in presenting it as a first-order formulation. The approach explicitly incorporates mechanical stress and coupled stress, with the former associated with spatial variations of rotation field.

Our contributions include identifying the operators in the Cosserat equations as a differential complex, termed the Cosserat complex. This complex is isomorphic to six copies of the de Rham complex, inherits its properties and establishes the L^2 version as the suitable framework for proving well-posedness. Additionally, we demonstrate the well-posedness of the first-order formulation through standard Ladyzhenskaya–Babuška–Brezzi (LBB) theory, revealing a connection to the Hellinger-Riessner formulation of elasticity with weak symmetry. This connection positions the Cosserat equations as a continuous extension of the elasticity equations.

Furthermore, we show that the two perspectives on well-posedness lead to distinct families of stable and convergent mixed-finite element discretizations, labeled as strongly coupled and weakly coupled, respectively. Notably, the non-conforming discretization remains stable in the continuous transition between Cosserat and elastic materials.

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Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTATIONAL MECHANICS OF GRANULAR MATERIALS WITH A LEVEL SET SHAPE DESCRIPTION

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ABSTRACT

In order to be quantitatively relevant, computational modeling of granular materials as per a Discrete Element Method (DEM) requires to either adopt an enriched contact model between spherical particles in the numerical world or a more faithful shape description of soil grains [1]. Among the various DEM implementations enabling the latter, a Level Set (LS)-based approach may implicitly describe grains shape through the zero-level set of the distance function to a grain surface [2,3]. Doing so, shape description starts by defining on a particle-centered grid appropriate values for the shortest distance to the grain, which is by convention taken to be positive outside of the particle and negative inside, while being naturally zero over its surface. Ensuring the versatility of the method, such a discrete distance field can be obtained for any surface through, e.g., a Fast Marching Method algorithm. For the purpose of contact detection, surface nodes furthermore discretize the particle boundary and can be obtained at will from the distance field. The method logically induces significant computational costs, be it either in terms of memory for the distance grid, or in terms of simulation time for looping over surface nodes when searching for an intersection with another particle (showing negative distance values in its inner region). The latter costs are carefully measured in the case of an implementation into the YADE code and discussed with respect to the obtained precision of the method. It is also shown how parallel, OpenMP, computing together with algorithmic improvements may help alleviating these costs, with a special focus on an optimized definition and manipulation of the surface nodes. This eventually enables the method to be conveniently applied to various cases stemming from convex superquadrics to non-convex rock aggregates.

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Geomechanics of the cryosphere
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DISCRETE ELEMENT SIMULATIONS OF SEA ICE IN TRIAXIAL TESTS UNDER DIFFERENT CONFINEMENTS AND BOUNDARY CONDITIONS

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ABSTRACT

ABSTRACT. The design of engineered structures in offshore areas in Arctic waters requires an estimation of the forces that can be produced by sea ice interacting with these structures. During an ice impact event, the load acting on the structure is transmitted through localized short-lived zones of intense high pressure along the contact surface, called high-pressure zones (HPZ). The sea ice experiences a complicated and random failure process over the HPZ. At the edge of the layer with relatively low pressures, microcracking and recrystallization are the primary failure mechanisms. In the central zone, with relatively high pressures, recrystallization and possible pressure melting influence the material properties of the ice materials. Due to the complexity and random nature of the ice failure over the HPZ, predicting the maximum ice pressure over time and its spatial distribution across the loaded area has been a challenge for researchers and practitioners. This paper presents a numerical model to quantify maximum sea ice pressure and to understand the effect of the ice state and characteristics. In particular, triaxial tests will be numerically simulated with spherical, bonded particles in a three-dimensional discrete element method-based PFC3D. Numerical simulation was performed for ice specimens subjected to vertical and radial stresses before shearing. After reaching an equilibrium state, shearing was simulated by applying incremental vertical displacements to the top wall. The flat-joint contact model was used for bonds between particles and the linear contact model was used for those between particles and the boundary walls. The model properly simulated the pre-failure behavior of sea ice. We characterized how boundary conditions (shape, stress, flexibility) and specimen packing (porosity and particle packing) affect macro- (strength or stiffness values and the post-peak behavior) and micro- (particle displacement and cracking) behavior of the sea ice. The model failed to capture the post-failure softening behavior of the sea ice. While sea ice under confinement is expected to exhibit strain-softening behavior in the post-failure range, the strength behavior of the sea ice in the numerical model changes abruptly to residual conditions more akin to brittle material behavior. We conclude that accurate prediction of sea ice’s post-failure behavior requires proper consideration of elastoplastic coupling for the degradation of elastic modulus with increasing plastic deformation.

Theory and application of provably-robust and efficient high-order methods for high-fidelity computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VORTICITY, ENERGY, AND ENTROPY CONSERVATION IN DG METHODS FOR THE SHALLOW WATER AND THERMAL SHALLOW WATER EQUATIONS

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ABSTRACT

We develop a novel structure preserving discontinuous Galerkin method for the shallow water and thermal shallow water equations in vector invariant form. The numerical method is nonlinearly stable and preserves important invariants in the system, including energy, vorticity, linear geostrophic balance, and buoyancy variance. These conservation properties are achieved by the discrete approximations on arbitrary curvilinear meshes through novel numerical fluxes and a skew symmetric formulation of the equations. Numerical experiments are presented to demonstrate the robustness of the method and verify the theoretical results on a cubed sphere mesh.

Immersed-boundary variational methods: Theory, data structures, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RECENT DEVELOPMENTS IN FINITE CELL ANALYSIS OF MICROSTRUCTURED MATERIALS

Alexander Düster[*1], Mahan Gorji[1], Seyed Farhad Hosseini[1], Lars Radtke[1] and Roman Sartorti[1]*

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ABSTRACT

Immersed-boundary methods and fictitious domain approaches are gaining popularity due to their ability to handle complex geometries without the need for body-conforming meshes. The finite cell method (FCM) is a combination of the fictitious domain approach with high-order finite elements. It offers the advantage of simplified pre-processing due to the use of Cartesian meshes. However, special attention must be paid to numerical integration, local refinement of the approximation, and the treatment of boundary conditions due to the non-conformity of the meshes to the problem's geometry.

This presentation will provide a brief overview of the finite cell method and showcase its applications in the structural analysis of microstructured, heterogeneous materials. These applications include the numerical treatment of material interfaces, fracture modeled by phase-fields, and simulation of acoustic properties of foamed material. The presentation will highlight the capabilities and challenges of the finite cell method in these contexts.

Lattice Boltzmann modelling and study of complex flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INFLUENCE OF PLASTICITY ON INERTIALESS VISCOELASTIC INSTABILITIES

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ABSTRACT

Many important practical applications involving porous media, cosmetics, biological systems, and food processing involve the transport of non-Newtonian fluids, which possess non-linear material properties. Elastoviscoplastic fluids are indeed a complex example, simultaneously involving viscous, elastic, and plastic properties. Purely elastic effects have previously been shown in viscoelastic fluids (i.e., solvent mixed with polymer additives) to transition the flow into a chaotic turbulent-like state, characterized by enhanced mixing, increased flow resistance, as well as strong flow fluctuations, even in the absence of inertia. In this study, we conduct numerical simulations of elastoviscoplastic fluids using a hybrid lattice Boltzmann solver in order to investigate the impact of plasticity, characterized by the Bingham number, on inertialess viscoelastic instabilities at high elastic effects. Notably, we investigate these effects across a range of different flow regimes. Results obtained using the four-roll mill and cellular-forcing scheme benchmark cases, which produce a strong elongational flow regime, reveal the emergence of three distinct flow states over time. The transition and behavior between the different flow states are found to strongly depend on the interplay between elasticity and plasticity. Moreover, we demonstrate that the general effect of the Bingham number in elongational flows is to increase the unyielded regions in the flow, which ultimately laminarize and suppress the flow fluctuations in the late stages. On the other hand, the unyielded regions in shear-dominated problems, such as the Kolmogorov flow, appear to enhance the turbulent characteristic of inertialess viscoelastic instabilities with increasing plasticity. Overall, the work presents preliminary results that demonstrate the contrasting effects of plasticity on inertialess viscoelastic instabilities depending on the flow type.

STABILIZED VIRTUAL ELEMENT METHOD FOR THE NONLINEAR CONVECTION-DIFFUSION-REACTION PROBLEM

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ABSTRACT

Convection-diffusion problems are of significant interest to both engineers as well as mathematicians. The Galerkin finite element approximation to this problem produces large non-physical oscillations and hence is unsuitable for this problem. This happens when the problem is either convection dominated and/or reaction-dominated. This drawback is addressed with the help of residual-based stabilization techniques such as streamline-upwind/Petrov-Galerkin (SUPG) and edge stabilization. In practical applications, the SUPG method produces inaccurate numerical solutions near the layers, and one needs to evaluate the second derivative when using high-order elements. To overcome this unwanted feature of SUPG methods, alternative methods are proposed and discussed in the literature, such as variational multiscale method, CIP method, orthogonal subscales method.

In this work, we have proposed and analyzed local projection stabilization for the virtual element discretization of the nonlinear convection-diffusion-reaction equation. A streamline-derivative-based stabilization is considered in the discretization of the model problem. This stabilization term is more general and preserves the stability property. We provide the existence of the discrete solution and then prove the optimal convergence rate in H^1 and L^2 norms, respectively. Numerical experiments show the better performance of the proposed VEM-LPS scheme compared with the gradient-based local projection stabilization method. The proposed method is more compact and offers the computational advantage that one need not compute the second-order derivative terms in the VEM-SUPG method.

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A PORT-REDUCED HYPERREDUCED REDUCED BASIS ELEMENT METHOD FOR MODEL REDUCTION OF COMPONENT-BASED NONLINEAR SYSTEMS

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ABSTRACT

This work introduces a reduced basis element (RBE) method for model reduction of parametrized, component-based systems in continuum mechanics governed by nonlinear partial differential equations (PDEs). The present work extends upon previous works on RBE methods for linear PDEs (e.g., [1]), which leverage the fact that many engineering structures consist of identical or similar components. In these approaches, a library of archetype components is created in the offline phase and is subsequently used in the online phase to build a reduced model for the systems instantiated from these pretrained components. While some extensions of the concept to nonlinear PDEs have been explored (e.g., [2]), they have been limited to systems with localizable nonlinearities or have not accommodated online interchangeable components.

To overcome these limitations, we present a port-reduced hyperreduced RBE (HRBE) method, which can handle global, nonlocalized nonlinearities and enables model reduction of large-scale problems with numerous continuous and topology-varying parameters. The primary ingredients of the method are as follows: an extension of the empirical quadrature procedure [3] to the component-wise reduced-basis construction and, in particular, hyperreduction of components; a library of archetype components comprising HRBEs of varying RB and hyperreduction fidelities; port-reduction, which provides a rapidly converging modal representation of solutions at component interfaces [1]; and an online adaptive scheme that is informed by the Brezzi-Rappaz-Raviart theorem and selects the appropriate HRBE fidelity for each component to meet the user-prescribe error tolerance at the system level in the online phase. We assess the formulation using large nonlinear hyperelasticity systems.

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Computational fluid dynamics (CFD) and fluid-structure interaction (CFSI): Methods and Applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A VERY HIGH-ORDER FRAMEWORK FOR FLUID STRUCTURE INTERACTION SIMULATIONS

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ABSTRACT

To accurately understand the complex flow phenomena surrounding machinery and structures, where fluid forces exert significant influence on the structures, fluid-structure interaction (FSI) simulations are crucial. These simulations consider the interaction between the fluid and structure, which is vital for analyzing the aerodynamic loads and the aeroelastic behaviour of the system. High-order, accurate, and cost-effective FSI methods are fundamental for improving the efficiency of existing structures or proposing new typologies and configurations. However, simulating body movements or relative motion of different parts while keeping computational costs low can be challenging.

The methodology proposed in this study combines the very high-order accuracy of the Finite Volume method based on Mean Preserving Moving Least Squares (FV-MP-MLS) [1] with the efficiency of the Chimera/overset grid framework [2, 3] to solve the Euler and Navier-Stokes equations. This approach offers a cost-effective solution for accurately analyzing and simulating fluid-structure interaction problems. The proposed method has been tested by solving a diverse set of benchmark problems, where the accuracy and performance of the method have been thoroughly evaluated and demonstrated.

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Data-driven approaches for solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEEP LEARNING FOR SURROGATE MATERIAL MODELING: CLASSICAL ELASTOPLASTICITY

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ABSTRACT

In this work, we present a deep neural network architecture specifically tailored for efficiently serving as a surrogate model for classical elastoplastic constitutive relations. The network is intricately enriched with essential physics principles inherent to classical elastoplasticity, encompassing the additive decomposition of strains into elastic and plastic components, alongside nonlinear incremental elasticity. This leads to a Physics-Informed Neural Network (PINN) model named here as Elasto-Plastic Neural Network (EPNN). Detailed analyses elucidate that incorporating these fundamental physics elements into the neural network architecture not only facilitates a more efficient training of the network with less training data, but also enhances the network's extrapolation capability to loading scenarios beyond the training dataset. The architecture of EPNN is model and material-independent, rendering it adaptable to a diverse array of elastoplastic material types, encompassing geomaterials. Moreover, the potential integration of experimental data directly into the network training process further extends its versatility. To showcase the robustness of our proposed architecture, we tailor its general framework to encapsulate the elastoplastic behavior of sands. Utilizing synthetic data derived from material point simulations based on an advanced dilatancy-based constitutive model for granular materials, we undertake the training of the neural network. The efficacy of EPNN is unequivocally demonstrated by its outperformance of conventional neural network architectures, particularly evident in its accurate prediction of unseen strain-controlled loading paths for sands exhibiting distinct initial densities. In essence, our work presents EPNN as a cutting-edge neural network architecture capable of efficiently emulating classical elastoplastic constitutive relations. The integration of crucial physics principles not only makes the network training more efficient, but also broadens the applicability of the model across diverse material types. The adaptability of EPNN to geomaterials, coupled with its potential utilization of experimental data, positions it as a powerful tool with far-reaching implications in the realm of computational material modeling.

Mechanics and physics of layer-like, fibrous materials and structures based thereon
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ELASTOPLASTICITY OF PAPER SHEETS: A CONTINUUM MICROMECHANICS APPROACH

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ABSTRACT

It is a well-known fact that paper materials exhibit elastoplastic behaviour. However, virtually all theoretical models that have been proposed to date are of the macromechanics (or “continuum”) type. Hence, the microstructural determinants of elastoplasticity in paper sheets remain elusive. Recently, some progress has been made in this regard, with a proposition based on continuum micromechanics and on extrapolation from elastic concentration relations and from a single fibre parameter covering complex elastoplastic events taking place at the microscopic scale at which fibres appear, being employed to theoretically predict the in-plane, ultimate strength of paper sheets [1]. However, the abovementioned single fibre parameter is a “black box”, so to say, having no direct relation with any experimental determinations related to the actual elastoplastic events. Accordingly, we herein go a step further in the process of fully connecting our theoretical model for the in-plane, ultimate strength of paper sheets with physically meaningful experimental determinations, and propose a much more sophisticated theoretical model relying on extensions to Dvorak’s classical transformation field analysis that make explicit consideration of plastic strains (in the form of eigenstresses), and which have recently been successfully used to address the elastoplastic behaviour of materials such as bones or rocks. Thereby, we reemploy large collections of experimental determinations that had been used to estimate volume fractions as well as other relevant quantities related to various, multiscale constituents of paper sheets made of softwood-based, unbeaten, chemical pulp fibres; and make use of several parameters related to a non-associated plasticity, to theoretically predict the complete stress-strain curve of the abovementioned variety of paper sheets [2]. Theoretically predicted relations between strain and stress up to ultimate strength agree outstandingly well with respective, experimentally determined curves [2]. These groundbreaking results open the way to more efficient and reliable, sustainable, theory-assisted, production, research and development, as well as use, of such materials.

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Machine learning algorithms for accelerating material characterization, discovery, design, and manufacturing processes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MACHINE LEARNING PREDICTION OF THE IMPACT OF H2O, NO2, SO2, AND H2S IMPURITIES ON THE CORROSION RATE OF CO2 TRANSPORT PIPELINES

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ABSTRACT

Despite significant efforts and investments in the renewable energy sector, fossil fuels continue to provide most of the world's energy supply. Transmission pipelines, extensively used in the oil and gas industry, are vulnerable to various failure mechanisms, such as corrosion. Corrosion control of gaseous CO2 transportation pipelines containing impurities such as water, H2S, NO2, and SO2 is important to the safe operation of pipelines. Correctly estimating the corrosion rate of CO2 transport pipelines helps to determine the allowable concentration of various impurities to estimate their integrity. This research provides a practical implementation of six machine-learning models for accurate internal corrosion rate prediction in oil and gas pipelines. Bagging Regression (BR), Ridge Regression (RR), Support Vector Regression (SVR), Random Forest (RF), Gradient Boosting Decision Tree (GBDT), and eXtreme Gradient Boosting (XGBoost) were among the predictive data models developed. These prediction models' implementation approach incorporates a comprehensive library of six system attributes from the literature. The significance of the input variables is determined through extra tree regressor feature importance selection criteria and statistical methods of feature selection using p-values with variance importance factor (VIF). Furthermore, k-fold cross-validation ensures good performance and generalization. The extreme gradient boosting model indicates the highest performance in predicting the internal corrosion rate of CO2 pipelines based on a mathematical RMSE score value of an internal corrosion rate of 0.031 mm/y. The results obtained were compared with experimental results from the literature and indicated the eXtreme Gradient Boosting model had the best performance with an R score of 0.885

Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE MODELING OF FRACTURE NUCLEATION AND PROPAGATION IN RATE-DEPENDENT POLYMER NETWORKS

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ABSTRACT

Materials with network-like microstructures, such as polymers, gels, and rubbers, are foundational in both natural and synthetic systems, including biological tissues, metamaterials, and soft robotics. Fracture processes in these materials are inherently multiscale and complex, necessitating advanced modeling techniques due to the computational challenges of fully discrete approaches in large-scale systems. We introduce an adaptive numerical algorithm, extending the Quasi-continuum (QC) method, to model fracture in networked materials with a focus on polymer networks. This method incorporates both material and geometric nonlinearities and employs a micro-macro energy consistency condition to achieve an anisotropic material tensor consistent with the network's underlying structure.

In areas of critical interest, such as near crack tips, we maintain an explicit representation of the local topology and represent each polymer chain as a nonlinear element governed by the worm-like chain model. Away from these imperfections, we limit the degrees of freedom and computationally homogenize the network structure. Our nonlinear finite element framework dynamically transitions between continuum and discrete scales, allowing for accurate modeling of crack propagation without a priori constraint on the fracture energy while maintaining the influence of large-scale elastic loading in the bulk

Expanding upon this methodology, we incorporate rate-dependent behavior into the QC approach to account for the viscoelastic behavior of polymer chains and dynamic bond breakage and formation. This includes a homogenization rule for the viscous forces and an updated adaptive mesh refinement algorithm. The framework's predictor-corrector scheme accurately resolves nodal displacements and velocities under varying loading conditions.

Our method demonstrates high accuracy and efficiency in modeling fracture in networked materials, as verified against fully discrete simulations. We explore the effects of network topology, disorder, and loading rates on fracture characteristics, highlighting the method's implications for multiscale analysis and discovery of new phase diagrams for crack patterns in viscoelastic systems. This extended approach offers a comprehensive tool for understanding and predicting fracture behavior in rate-dependent polymer networks.

Inverse and optimization problems for advanced materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION WITH STOCHASTIC GEOMETRIC PERTURBATIONS FOR WAVEGUIDE DESIGN

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ABSTRACT

Uncertainties in manufacturing processes are found everywhere in industry and for this reason devices usually operate with tolerances. But some products are so sensitive that even small perturbation alters their performance dramatically. Such devices are often found in compliant mechanisms or wave propagation problems, e.g. propagation of elastic-, acoustic- or electromagnetic waves, where a small perturbation of the device geometry can easily degrade performance significantly.

Standard topology optimization approaches including geometric uncertainties through robust formulation exist, e.g. in [1] for acoustic waves and [2] for mechanics, using an over- / under etching technique. The standard approach is computationally heavy and perturbation methods have been tried [3] but encountered challenges for large material contrasts as found in e.g. structural problems.

This study build on the knowledge in [3] but for an optical problem, which has a high chance of showing good results due to smaller material contrasts. The method emulates perturbations of the design caused by fabrication, such as electron beam lithography, using stochastic fields. A design robust to the specified variation results directly from the optimization with performance assigned a mean and standard deviation. The method only requires a single factorization of the system matrix per iteration, whereas standard robust topology optimization techniques [1, 2] requires multiple.
This study optimizes optical waveguides, which are used as components in larger circuits. Within the variations assumed for the manufacturing process, a robust optical waveguide is demonstrated to appear from the optimization. Having knowledge of the natural variation in performance helps us assess the performance of other components in the circuit, or the entire circuit itself. Other applications will include slow-light and extreme dielectric confinement waveguides.

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Geometric mechanics formulations and structure-preserving discretizations for continuum mechanics and kinetic models
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STRUCTURE-PRESERVING, HIGH-ORDER, OSCILLATION-LIMITING, BOUNDS-PRESERVING (SPHOOL-BP) TRANSPORT OPERATORS FOR ARBITRARY K-FORMS USING DISCRETE EXTERIOR CALCULUS

Christopher Eldred[*1]*

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ABSTRACT

Many fluid dynamical systems can be described by a (convective) velocity and a set of state quantities such as mass density, specific entropy and electromagnetic fields, etc. When the dynamics are reversible and the state quantities are advected (their behavior is governed entirely by a Lie derivative), then the resulting set of equations have a special semi-direct product structure that leads to a Lie-Poisson Hamiltonian formulation (or equivalent forms obtained through a change of variables such as Curl-Form). In these formulations, each advected quantity induces a corresponding term in the momentum equation, governed by a diamond operator.

In this talk we will discuss the development of structure-preserving, high-order, oscillation-limiting, bounds-preserving (SPHOOL-BP) transport operators using discrete exterior calculus (DEC) for state quantities that are scalar-valued differential k-forms (SVDFs), including discrete versions of both Lie derivatives and diamond operators. This builds on previous work for \scalar-valued volume forms such as mass density or entropy density, extending it to arbitrary scalar-valued k-forms such as electromagnetic fields or specific entropy.

SPHOOL-BP transport operators offer: (1) preservation of geometric mechanics structure, in particular anti-symmetry of the Poisson bracket needed for energy conservation; (2) high-order accuracy in smooth regions and high-resolution in regions of sharp gradients or discontinuities; (3) oscillation-limiting through WENO or related reconstructions; and (4) (local) bounds-preservation through flux corrected transport.

If time permits, there will be discussion of preliminary work on how to extend these ideas to arbitrary (vector) bundle-valued differential forms (BVDFs), which would be required to treat quantities such as fluid momentum or tensor order parameters in models with fluid microstructure.

GROUP ESTIMATORS FOR MULTIFIDELITY SAMPLING

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ABSTRACT

Multifidelity uncertainty quantification can be an effective tool for quantifying the effects of statistical variability for physics simulations that require expensive high-fidelity computational models. By optimizing the allocation of computational resources among multiple models of varying accuracy and cost, accurate estimates of statistical quantities of interest can be obtained at significantly lower cost than for single-fidelity approaches. Recent work has explored refinements that aid in the practical deployments of multifidelity sampling methods, including iterated pilot management, selection of the most performant approximation memberships and relationships (ensemble and DAG selection), and hyper-parameter model tuning. These refinements target the full set of available sampling estimators, but have been observed to be most effective given the addition configuration freedom in non-hierarchical cases, i.e. in approximate control variate (ACV), generalized ACV, and multilevel best linear unbiased estimator (ML BLUE) contexts.

In this work, we dive deeper into group estimators, including ML BLUE and recent extensions which seek to relax certain constraints enforced in the ML BLUE formulation. Group formulations can directly facilitate ensemble selection using semi-definite approaches to resource allocation, and we seek to augment this capability with effective approaches for online/offline pilot management and hyper-parameter model tuning.

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Isogeometric methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FAST SPACE-TIME ISOGEOMETRIC SOLVERS FOR THERMO-MECHANICAL PROBLEMS

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ABSTRACT

IsoGeometric Analysis was introduced as an “extension” of Finite Element Methods which obtains better results by increasing the polynomial degree p and refining the mesh size h. However, its application implies great computational challenges since the cost increases rapidly with the degree p. This communication focuses on novel techniques like Matrix-Free and Fast Diagonalizationmethods which, coupled with IGA, enable to:
• reduce storage memory and computation time by not constructing/storing the matrices but instead using an iterative solver with efficient matrix-vector products;
• enhance the convergence rate of the Krylov solver by introducing an inexpensive, easy to code and effective preconditioner.
The objective of this communication is to illustrate the synergy between these approaches applied to space and space-time problems considering heat transfer and elasto-plasticity. We will show that the proposed method will illustrate significant cost reductions.

Novel mathematical and numerical models for multiphysics and multiscale systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HIGH-ORDER DG METHODS FOR THE CELL-BY-CELL ELECTRONEUTRAL NERNST-PLANCK FRAMEWORK

Ada Johanne Ellingsrud[*1] and Miroslav Kuchta*[1]

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ABSTRACT

Despite the fundamental role of movements of molecules and ions in and between cellular compartments for brain function [1], most computational models for excitable tissue assume constant ion concentrations. Although these models have provided valuable insight into how neurons function and communicate, they fail to describe vital processes related to signalling and brain homeostasis, and pathologies involving substantial changes in the extracellular ion composition such as epilepsy and spreading depression.

Here, we discuss the emerging KNP–EMI framework [2], describing the coupling of ion concentration dynamics and electrical properties in excitable tissue with explicit representation of the cells, allowing for morphologically detailed descriptions of the neuropil. In contrast to classical homogenized models, the highly detailed KNP-EMI framework enables modelling of single cells and small collections of cells, uneven distributions of membrane mechanisms, and how the cellular morphology affects tissue dynamics.

The system consists of non-linear, highly coupled, and mixed-dimensional partial differential equations. Numerical strategies for approximating the system must as such be chosen with care. We present a novel numerical strategy with three key components: (i) a splitting scheme to decouple the PN equations governing ionic transport and the equation arising from the electro-neutrality assumption, (ii) a high-order Discontinuous Galerkin (DG) discretization of the decoupled system, and (iii) a robust and scalable solver. We further analyse and discuss stability and convergence properties of the proposed scheme, and show that our solution approach is robust and scalable allowing for large-scale, high-realism in-silico studies of electrodiffusive processes in excitable tissues.

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Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MESHFREE FRAGMENTATION AND ANALYSIS OF MASS DISTRIBUTIONS FROM EXPLOSIVE EVENTS

William Elmer[1] and Colton Ross*[1]

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ABSTRACT

Meshfree Fragmentation and Analysis of Mass Distribution from Explosive Events.
Aug. July 21-26, Advances and applications in meshfree, particle, and peridynamic methods, in Conference: WCCM 2024/PANACM 2024, Vancouver, Canada.

Meshfree methods appear to be well suited for problems involving fragmentation because no mass is lost in the service of preserving numerical stability under extreme deformation, i.e. meshfree methods do not require element deletion. Natural fragmentation is the process by which solid bodies, subject to extreme events like hypervelocity impact or explosive loading, fracture into small pieces of material. Robust treatment of fracture is necessary for capturing the resulting mass distribution of fragments because fragmentation is a race between the ongoing loading of the structure and unloading caused by fracture (1).

However, despite the apparent benefits of Meshfree methods, computational methods used to generate fragments are limited not only by the mesh resolution, but also inaccuracies as fragments approach this size. Numerical techniques that accommodate failure and fragmentation typically maintain conservation of mass and momentum by forming particles or “fragments” on the order of the mesh discretization. “Fragments” that are generated below a certain size cease to encode relevant information about the physics of the explosive event, and instead represent a-priori construction of the mesh. We will study the role of statistical damage seeding, relation to static failure tests, and mesh resolution.

Using a previously developed technique (2) for the quantitative comparison between explosive events that generate fragments, comparisons will be shown between empirical pipe-bomb events numerical simulations from ALE3D utilizing the meshfree SPH formulation Spheral (3). We use the method (2) to assess the suitability of different numerical methods to calculate observed fragment sizes within the bounds established by experiment. The empirical dataset contains a test matrix of two different high explosives with high and low brisance, and three heat-treatments of 4340 steel: displaying a 50% variation in elastic modulus and a 57% variation in ultimate tensile strength.

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Data-driven modeling and design of materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DISCOVERY OF COMPOSITE MATERIAL ARCHITECTURES USING PERPETUAL MACHINE LEARNING

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ABSTRACT

Architectured materials, such as composites, gives the designer the ability to tailor a material's performance to each specific structural application. These materials often exhibit strong heterogeneity manifesting as coupling between the material internal architectures and the structural geometry. Examples of this behaviour can be seen in 3D woven composites and tow steered composites, where the fibre paths are dependent on the structural geometric features, but also the manufacturing methods used. As a result, complex and computationally expensive multi-scale and multi-physics simulations are often needed to predict the mechanical performance on the structural scale, as well as the impact of manufacturing methods on the material architecture. While these models are very effective as analysis tools, their prohibitive computational cost make them unsuitable for design and optimisation tasks. Multi-scale data-driven approaches has seen wide use in optimisation and design of such structures. This is often achieved by sampling the material design space in advance and building a surrogate model to represent the materials' response as a function of their architecture, which is later used in design/ optimisation. However, with large scale structure and complex material architectures, this sampling process is often very expensive and time consuming.

In this work, a novel approach based on perpetual machine learning is introduced. This approach enables the simultaneous discovery and optimisation of material architectures, structural geometries, and accurate multiscale representations of both. The perpetual learning framework continuously trains two machine learning models, a classifier representing a given problem constraints such as the occurrence of failure or structural buckling, and a surrogate model representing the structural behaviour inside the design space. The discovery process is carried out in an iterative manner, where in each iteration an optimiser finds an interim optimal point based on information from the surrogate model and the classifier. Following, the training database is enriched using multi-scale simulations at key test points, chosen based on the confidence margins of the classifier and surrogate model, as well as the interim optimal solution. Using this iterative process, the framework continually samples the material and structure design space to develop a better description of the structural response and the conditions at which failure might occur. The proposed approach has demonstrated the ability to discover machine learning models for a variety of analytical problems and realistic composite material and structures.

Fluid dynamics and SciML: Navigating challenges and seizing opportunities
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ACTIVE CONTROL OF FLUID-STRUCTURE INTERACTION SYSTEMS USING DEEP REINFORCEMENT LEARNING

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ABSTRACT

This study introduces an innovative deep reinforcement learning (DRL) approach for the active control of fluid-structure interaction (FSI) in a laminar flow environment. Focusing on active flow manipulations using actuators within FSI systems, we develop effective control policies for the displacement control of the simulated structures. For the simulations, we rely on an open-source coupling library for partitioned multi-physics simulations (preCICE), integrated within the reinforcement learning Gym-preCICE framework. The uniqueness of this research lies in using the Proximal Policy Optimization (PPO) algorithm, a state-of-the-art on-policy DRL method, to actively control the system using a predefined reward function.

To the best of authors' knowledge, this research represents the first attempt to use DRL for active control of complex FSI scenarios involving 2D dynamics of rigid (Vortex-Induced-Vibration, VIV) and flexible (Fluid-Induced-Deformation, FID) bodies. Our results show that the DRL-controlled system, employing the PPO algorithm, can adaptively and efficiently control FSI systems, offering a superior alternative to traditional control methods. This approach holds significant potential for applications in engineering structures where FSI is a primary concern, such as in bridge aerodynamics, marine structures, and wind turbines. Future work will aim to expand the scope of this method to include more dynamic and realistic FSI scenarios, potentially revolutionizing how FSI phenomena are addressed in various engineering applications.

Keywords: Fluid-structure interaction (FSI), Deep reinforcement learning (DRL), Active flow control (AFC), Gym-preCICE, Proximal Policy Optimization (PPO)

Buckling analysis and design of thin-walled structures based on novel and intelligent computational methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTATIONAL MODEL FOR LOCAL BUCKLING OF COMPRESSIVELY LOADED OMEGA-STRINGER-STIFFENED PANELS

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ABSTRACT

Thin-walled composite structures are used in applications such as aircraft and spacecraft due to their low weight and corresponding high stiffness properties. To optimize the potential of these structures to the fullest extent, a complete understanding of their stability behavior is required. Thereby, uniaxial compression describes an important load case that is investigated. A closed-form analytical method based on the energy method for determining the local buckling load of omega-stringer-stiffened panels is presented. The stiffened panel under consideration consists of the skin plate with eccentrically attached stringer feet along the longitudinal sides of the panel, while the remaining part of the omega-stringer is modeled by corresponding elastically restrained edges. Due to the applied stringer feet, stiffness discontinuities occur in the stiffened panel. This is covered by the presented method, whereas in comparable studies in the literature, a homogeneous stiffness is often assumed across the entire panel. To evaluate the new analysis method, a comparison with the numerical solution of the corresponding Lévy-type solution and the finite element analysis is being drawn.

Advanced analysis of steel and steel-concrete composite structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FATIGUE PROPERTY OF STEEL-CONCRETE COMPOSITE BEAMS UNDER SAGGING MOMENTS

Ayman Elzohairy[*1], Hani Salim[2] and Hesham Shaaban[3]*

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[3]*Zagazig University*

ABSTRACT

Superstructures of bridges are susceptible to fatigue loading when subjected to service loads, potentially leading to premature structural failure. This study presents experimental findings obtained from fatigue loading tests conducted on composite beams with various configurations. These fatigue tests involved subjecting the beams to one million cycles of four-point loading with varying shear stress ranges at a consistent amplitude. Additionally, the research investigated the influence of external post-tensioning and the strength of the shear connection. In order to evaluate the residual strength of the fatigued specimens, static tests were performed until failure. Throughout the testing process, we monitored mid-span deflections, slippages between concrete slabs and steel beams, strains in the shear connectors, and strains in the concrete slabs and steel beams. The experimental results revealed that as the number of cycles increased, the shear studs caused damage to the concrete slab, resulting in a loss of stiffness in the shear connection. This led to increased residual deflections and plastic slippages. The control of longitudinal fatigue cracks in the concrete slab was largely dependent on the strength of the shear connection between the steel beams and concrete slabs. Additionally, the shear stress range in the shear connectors influenced the formation and distribution of fatigue cracks in the concrete slab. Furthermore, the application of external post-tensioning significantly reduced the strains in the steel beam, concrete slab, and shear connectors. Remarkably, the tendons displayed excellent fatigue performance with no signs of distress at the anchors.

Advanced materials and smart structures: Modeling, simulation and testing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DESIGN OF ACOUSTIC METASURFACES FOR LOUVERS OF ENGINE ROOM USING TOPOLOGY OPTIMIZATION CONSIDERING VISCOSITY AND TEMPERATURE BOUNDARY LAYERS

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ABSTRACT

Sound radiation from the engine compartment louvers of construction machinery and automobiles poses a significant noise pollution challenge to urban residents and others. To address this problem, we used topology optimization to design an acoustic metasurface specifically tailored as a louver structure. This design strategically directs sound from its source in selected directions, regardless of the direction of the incident sound. The optimization process employed the Sequential Linearized Navier-Stokes model, which meticulously accounts for the effects of viscous and thermal boundary layers using the level set method. A comparative analysis was performed to evaluate the impact of these boundary layer effects on the optimization results. The mechanism of the optimized structure was rigorously modeled, and its frequency response was numerically analyzed. This analysis revealed that the response depends on the specific dimensions of the structure. Based on these findings, we proposed a simplified version of the louver structure designed for ease of fabrication. The performance of this streamlined structure was then numerically validated, demonstrating its potential effectiveness in mitigating urban noise pollution.

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Quantum scientific computing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PROPOSING OF NOVEL REAL NUMBER REPRESENTATIONS IN ISING MACHINES

Katsuhiro Endo[*1], Yoshiki Matsuda[2], Shu Tanaka[3] and Mayu Muramatsu[3]*

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ABSTRACT

Quantum annealing machines are attracting attention as next-generation solvers to solve combinatorial optimization problems. Physics simulation can be one of the useful areas where quantum annealing machines can be applied. It is because some physical phenomena are simulated to find minimum energy states, and quantum annealing machines accelerates to find them as combinatorial optimization problems. It could also be used to optimize the initial conditions for better results.

In this study, we focus on a method of representing real numbers using binary variables, or quantum bits. To use a quantum annealing machine, all problems must be converted to combinatorial optimization problems of binary variables. On the other hand, since general physics simulation problems involve real numbers in the decision variables, real numbers must be expressed as a combination of binary variables. We have found that the method of representation of real numbers causes a significant change in the quality of the results obtained by the quantum annealing machine. We also find that the most appropriate representation method depends on the size and difficulty of the problem to be solved, and that these differences show consistent trends across the two annealing solvers. Finally, we explain the reasons for these differences using a simple model, the minimum number of simultaneous bitflips required, and one-way stochastic bitflip energy minimization.

Certification of simulations and model adaptation in computational science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BOUNDS FOR GOAL ORIENTED ERROR ESTIMATION

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ABSTRACT

In many applications, the primary focus is not on solving the partial differential equation but rather on a quantity of interest that depends on the solution. In this talk, we will derive goal-oriented error estimation and mesh adaptivity for this quantity of interest. This process requires either a hierarchical approach or interpolation. We will provide efficiency and reliability results for both, assuming that a saturation assumption for the quantity of interest is met. Here, both the partial differential equation and the quantity of interest may be nonlinear. In conclusion, the numerical findings will be supported by numerical examples.

Biomechanics of hard tissues: From experiments and simulations to clinical applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTATIONAL AND EXPERIMENTAL CHARACTERIZATION OF FUNCTIONALLY GRADIENT BONE TISSUE SCAFFOLDS FOR COMPLEX LOADING CONDITIONS

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ABSTRACT

Structures with Triply Periodic Minimal Surfaces (TPMS) have gained significance for various applications in biomedical engineering, including tissue scaffolds. TPMS bone tissue scaffolds possess interconnected pores and a large surface area, which can facilitate cell adhesion and nutrient diffusion. To enhance the biomimetic nature of these TPMS scaffolds, functional gradients such as pore size and porosity variations are often incorporated into these scaffolds. While functionally gradient scaffolds have been shown to achieve better bone regeneration outcomes, variations in their pore size and porosity distributions can significantly influence their mechanical behaviour, which needs to be carefully considered when designing these structures. Recent studies have investigated the mechanical characteristics of functionally gradient scaffolds under axial loading. However, bone scaffolds usually undergo far more complex loading conditions, including compression, shear, and torsion. Hence, the mechanical behaviour of these scaffolds must be investigated in various loading scenarios to ensure their efficacy in real-world applications.

This study systematically investigates the mechanical properties of functionally gradient TPMS structures in various loading conditions. Two different TPMS scaffolds, including gyroid and primitive, are designed with various porosity distributions while the overall porosity is kept constant between all groups. Finite element analysis (FEA) is conducted on each scaffold with a cylindrical shape to evaluate their stress distribution, stiffness, and strength under three different loading scenarios, including compression, shear, and torsion. To validate the FEA results, the scaffolds are fabricated from Acrylonitrile butadiene styrene (ABS) using PolyJet™ 3D printing technique. Then, in-house experimental mechanical tests are conducted on the scaffolds using customized jigs to replicate the loading conditions used in the FEA simulations. The computational results indicate that a decrease in the porosity of the scaffolds toward their centre can significantly enhance their stiffness and strength. Moreover, it is demonstrated that a sharper decrease in porosity can further increase the stiffness and strength of the scaffolds. Furthermore, the FEA results are validated by our in-house experimental data obtained from the compression, shear, and torsion testing on the scaffolds.

This study concluded that TPMS structures with functionally gradient pore size and porosity could significantly improve the mechanical properties of bone scaffolds in complex loading conditions. Moreover, the rate of variation in the pore size and porosity distribution could further control the mechanical behaviour of these porous structures. This study is expected to provide significant insight into the design of functionally gradient structures for applications in tissue engineering and bone implants.

Nanomechanics and nanoscale thermal transport for new materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ATOMISTIC SIMULATIONS OF DIFFUSION PROCESS IN MATERIALS SUBJECT TO EXTREME CONDITIONS

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ABSTRACT

To explore various physical and chemical phenomena at the nanoscale, in which materials often exhibit properties divergent from their bulk counterparts, atomistic modelling tools prove more advantageous than the traditional thermodynamic approach. Among them, Molecular Dynamics (MD) simulations stand out as a pivotal and influential tool, offering an in-depth exploration of physical phenomena within nanostructures at the molecular level. MD simulations enable the precise prediction of atom trajectories within molecular systems, guided by interatomic potentials, thereby facilitating a profound understanding of nanostructure evolution. This includes elucidating the elusive atomistic intricacies of diffusion phenomena, which are often challenging to observe both experimentally and through a thermodynamic approach.

In this study we aim to explore physical and chemical phenomena at the nanoscale, in which materials often exhibit properties divergent from their bulk counterparts. We will employ MD simulations to characterize mutual diffusion behavior, as well as the intricate structure and evolution processes of bimetal systems at their interfaces and our overarching goal is to undertake a comprehensive exploration of diffusion phenomena at bimetallic interfaces, spanning diverse film-substrate systems. Employing advanced machine learning methods, including data dimension reduction techniques and neural network, our aim is to identify the optimal multimetal film compositions with the best diffusion properties and to enhance our understanding of the fundamental principles governing the phenomena.

We will consider factors such as cohesive energy, surface energy, atomic size, and electronegativity, as the features (descriptors) in the machine learning. We will also investigate chemical reactions occurring within the film-substrate systems, facilitated by, for example, carbon and oxygen, and how the newly formed species act as diffusion barriers. This exploration will entail the use of reactive molecular dynamics using ReaxFF potential.

Furthermore, we will investigate the chemical reactions occurring within thin films, particularly in conjunction with carbon and oxygen, and how the newly formed species act as diffusion barriers. We present simulation of diffusion behavior for various multimetallic film-substrate combinations using MD approach and predict the optimal metallic combinations for the film using neural network. In addition our simulation will add the effect of chemical reactions on the diffusion process and we will develop a methodology for a holistic understanding of interdiffusion mechanisms in multimetallic structures at the atomic level.

Recent advances in indirect structural health monitoring
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STABILITY ENHANCEMENT THROUGH REALTIME-OPTIMIZATION OF MOBILE DEVICE-BASED VIBRATION MEASUREMENT

Sung-min Eom[1], Daeho Nam[2], Hwan-youp Oh[2], Hye Young Jo[2], Kyung-ho Sun[3] and Yun-ho Shin[1]*

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ABSTRACT

Vibration measurement during ship trials is crucial for safety and the lifespan of structures. However, field engineers often face challenges in accurately measuring vibrations due to various difficult environments. In response, the industry has increasingly demanded a flexible, accurate, and stable vibration measurement tool. Our research has developed a mobile-based vibration processing system using image processing techniques. A key method employed is the phase correlation-based template matching, known for its effectiveness in vibration measurement. This approach involves extracting the Region of Interest (ROI) and comparing phases to determine changes in vibration. A major focus of this study has been on mitigating the variability in measurement accuracy due to the way the ROI is established. As a result, we have conducted research and development focused on optimizing the placement of ROI for improved accuracy in vibration measurement. Additionally, this study has analyzed the challenges encountered during sea trials on real ships, focusing on deriving results from actual vibration measurements. These analyses included identifying environmental factors that negatively impact the accuracy and reliability of these measurements. We identified and categorized various factors that could potentially impact the results and identified those with the most significant influence. This process helped us determine which aspects to focus on for in-depth analysis before proposing solutions.

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Applications of shape optimization in complex engineering problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ACOUSTIC SHAPE OPTIMIZATION USING ENERGY STABLE CURVILINEAR FINITE DIFFERENCES

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ABSTRACT

It is well known that high-order finite difference methods (HOFDM) are well suited for long-time simulations of wave propagation problems. An established approach for obtaining efficient and robust HOFDM is to discretize in space using schemes satisfying a summation-by-parts property [1]. Summation-by-parts finite difference operators are designed to satisfy a discrete version of integration-by-parts, allowing for semi-discrete energy estimates that mimic the equations in the continuous setting. This leads to provably stable high-order schemes that can be implemented with the computational efficiency typical of finite difference methods.

Historically, summation-by-parts finite differences have mostly been used to obtain approximate solutions to partial differential equations (the forward problem). In this work (see preprint in [2]), we apply the summation-by-parts finite difference method to shape optimization problems constrained by the acoustic wave equation. The new approach makes use of state-of-the-art summation-by-parts finite difference techniques together with a gradient-based method to obtain an efficient solver for the shape optimization problem. Representing the design domain through a coordinate mapping from a reference domain, the design shape is obtained by inversion of the discretized coordinate map. The adjoint state framework is employed to efficiently compute the gradient of the loss functional.

Using the summation-by-parts properties of the finite difference discretization, we prove stability and dual consistency of the semi-discrete forward and adjoint problems. This means that the "discretize-then-optimize" and "optimize-then-discretize" approaches are equivalent for this problem. We also verify the accuracy of the finite difference scheme numerically and demonstrate the capabilities of the shape optimization method by solving two two-dimensional model problems with real-world relevance. First a bathymetry problem (determining the shape of ocean floors) and then the problem of optimizing the shape of an acoustic horn to minimize the reflected sound.

In my talk I will present the basic ideas behind summation-by-parts finite differences, our approach to the shape optimization problems, and numerical experiments demonstrating the capabilities of the method.

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Advance modeling and simulation in complex porous media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFECT OF TUBE-TO-PARTICLE DIAMETER RATIO ON THE FRICTION FACTOR FOR AIRFLOW INSIDE A PACKED BED OF PARTICLES: PORE-SCALE NUMERICAL MODELING

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ABSTRACT

Packed beds find various industrial applications such as catalytic reactors, filtration and separation, food processing as well some niche applications in mining like heap leaching and underground thermal energy storage. One of the most critical design parameters in packed beds is the pressure drop along the bed, often characterized by the friction factor coefficient. Although many correlations are readily available relating the friction factor to the flow Reynolds number (Rem), the impact of critical factors such as particle shape, size distribution, and tube-to-particle diameter ratio (N) on the friction factor remains less explored. Some authors have proposed correlations including sphericity for particle shape and an equivalent diameter for size distribution, yet there is no clear consensus on how tube-to-particle diameter ratio can be taken into account in friction factor correlation. This study investigates the effect of tube-to-particle diameter ratio and assess the validity of available correlations on finite beds with low N values. Pore-scale modeling based on particle-resolved Computational Fluid Dynamics (CFD) is performed to study the airflow dynamics within the packed bed of rocks, offering a detailed examination of the fluid dynamics at microscopic level. These findings underscore the necessity to revisit existing correlations in friction factor assessments, bringing attention to the nuanced role of N in the determination of pressure drop in packed bed of particles.

Multiphysics and data-driven modeling for cardiovascular biomedicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A DATA-DRIVEN REDUCED ORDER MODEL OF FLUID FLOW WITHIN A FEMORAL VEIN

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ABSTRACT

Venous thromboembolism (VTE), including Deep Vein Thrombosis (DVT) and Pulmonary Embolism (PE), are two major cardiovascular diseases worldwide [1]. Deep vein thrombosis and pulmonary embolism impose more than $10 billion/year economic burden on the USA's health system [1]. Therapeutic methods that are commonly used to treat DVT include anticoagulant medication, catheter-directed intra-thrombus thrombolysis (CDIT), Inferior Vena Cava (IVC) filter, pharmacomechanical catheter-directed thrombolysis (PCDT), percutaneous mechanical thrombectomy (PMT), and ultrasound catheter-based thrombolysis [2,3]. Anticoagulants such as heparin, warfarin, and blood thinners are prescribed to prevent or resolve venous thrombi by interrupting the clotting cascade. Anticoagulant therapy increases the risk of bleeding, impacts the coagulation cascade in the whole body, and is less effective due to the longer time of clot dissolution. IVC filters, CDIT, PMT, PCDT, and ultrasound are localized methods to dissolve or physically remove the clot, offering potentially higher efficiency compared to anticoagulants. However, these methods are invasive and may lead to an increased risk of stroke, embolization, perforation, and thrombosis. To address the limitations of current thrombus management techniques, it is crucial to predict the risk of DVT and develop non-invasive thrombolysis methods. A fluid dynamic model integrated with a coagulation cascade model is required to predict the risk of DVT. The time required to solve full-order FSI and CFD models is much higher than the actual time taken for thrombus formation. Therefore, it is challenging to apply full-order CFD and FSI models to predict the DVT before it occurs. We developed a reduced order model (ROM) of flow within deep vein valves to reduce the computational time related to solving Navier-Stokes and structural mechanics equations. We fabricated five femoral vein silicone phantoms and placed them in a flow loop to record the leaflet displacement, wall shear stress, velocity vectors, and pressure data using a particle image velocimetry system (PIV). We tested the flow under various heart rates. These data were stored as a snapshot library to develop a ROM FSI. Using proper Orthogonal Decompositions (POD)-Galerkin, the FSI governing equations were projected into the ROM basis and then were solved. The ROM model developed in this work is five times faster than using a full-order FSI simulation to model blood flow within a femoral vein.

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HYBRID STRUCTURE HEALTH MONITORING TECHNIQUE FOR ENHANCING MODAL PARAMETER IDENTIFICATION ACCURACY

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ABSTRACT

SHM relies on the possibility of estimating structural modal parameters, such as mode shapes, natural frequencies, and damping, from the structure's measured data. Nevertheless, modal parameter estimation still faces accuracy problems. Traditionally, measured data were obtained by instrumenting bridge structures with connected sensor systems which faced many technical problems such as high cost, maintenance issues, safety, and traffic disruption among others. Later, a practice shift favored indirect SHM (iSHM) methods among which drive-by using passing instrumented vehicle is well researched [1,2]. These methods still don't solve the problem with modal parameters identification accuracy especially higher mode of vibration believed to be sensitive to localized bridge damage which limits the widespread adoption of iSHM methodologies [1,3]. A combination of the two prominent methodologies is proposed to address the limitations of existing methods by combining the advantages of indirect monitoring and direct monitoring. This is thought to improve the modal parameters identification including the higher modes of vibration for localized damage detection and structural assessment.
The proposed approach uses GPS-time synchronized sensors to ease the simultaneous measurement of vehicle and bridge vibration data. Furthermore, the proposed method is verified by numerical simulation assuming a multi-run scenario over the same bridge. The key findings of this study highlight the potential of the hybrid SHM technique in significantly improving the accuracy of indirect structural health monitoring. The results demonstrate that the integrated approach outperforms the existing methods by providing more reliable and precise modal parameter estimates, especially higher modes of vibration, allowing the identification of the bridge's localized damage.
Keywords: Hybrid structure health monitoring, GPS clock synchronization, modal parameters identification.

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Efficient iterative methods for solving coupled and strongly nonlinear problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NONLINEAR CONJUGATE GRADIENT SOLVERS FOR LARGE DEFORMATION NONLINEAR FINITE ELEMENT MODELS

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ABSTRACT

Although finite elements are widely used for large deformation, nonlinear problems, conventional solvers using BFGS quasi-Newton or similar methods are often slow and frustratingly unreliable, especially where severe nonlinearities such as buckling are present. The size of models that can be solved is limited by the memory required for the tangent stiffness matrix. Explicit solvers are increasingly widely used to try to avoid these problems, but can also be frustratingly slow, especially for quasistatic problems. Direct solution using nonlinear conjugate gradient methods is an interesting alternative that could perform much better for large, highly nonlinear problems.

A nonlinear conjugate gradient solver using the Hager-Zhang CG-DESCENT algorithm with a modified linesearch was implemented in the FEBio software package. Various test models were used to benchmark the algorithm against the standard BFGS solver.

For small models the conjugate gradient algorithm was significantly slower, but for large models it was up to two orders of magnitude faster for moderately nonlinear models. It was also able to solve models an order of magnitude larger. For highly nonlinear models that were difficult or impossible to solve using the BFGS solver, the conjugate gradient algorithm converged reliably, often in a single timestep, although this often required a long solution time.

Because displacements propagate slowly across the mesh over many iterations, prescribed displacement boundary conditions can cause excessive mesh distortion and must be applied with care. However, inadequate constraints do not cause large and uncontrolled displacements as they do with Newton-Raphson solvers, which is very helpful for multibody contacts and similar problems.

Where different nodes have significantly different stiffnesses, for example for different materials or midside nodes in quadratic elements, some nodes can move faster than others during the solution causing mesh distortion. This can be alleviated by using a preconditioner, for example the main diagonal of the tangent stiffness matrix, although in general this did not consistently improve the performance of the algorithm. No doubt better preconditioners could give significant performance improvements.

In summary, nonlinear conjugate gradient algorithms have considerable potential for large, highly nonlinear problems and there is great potential to develop them further.

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Probabilistic learning and constrained generative models for uncertainty quantification
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PROBABILISTIC LEARNING IN NONLINEAR COMPUTATIONAL STOCHASTIC DYNAMICS: INVESTIGATING A PARTIALLY OBSERVED UNCERTAIN NOZZLE MODEL

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ABSTRACT

This papers deals with the numerical application of the Probabilistic Learning on Manifold (PLoM) method to construct a statistical surrogate model consistent with a small and incomplete target dataset. The structure under consideration is a three-dimensional engine nozzle, made up of an homogenized elastic material and subjected to random internal pressure excitation. The dynamical model assumes large displacements. A target dataset is assumed to be given, which is constituted of a subset of the normal displacements located in the nozzle exit, and expressed in the frequency domain. These random frequency response functions form a subset of the Quantities of Interest (QoI) that will be considered as the model outputs. A parameterized Stochastic NonLinear Computational Model (SNLCM) representing the nozzle dynamics is constructed. Its control parameters describe the power spectral density of the stochastic excitation force. Furthermore, the elasticity matrix is homogeneous, anisotropic and random, whose mean value corresponds to an isotropic elasticity matrix. Due to the complexities of such a nonlinear computational model, the calculation of the dynamical response for a given set of parameters induces a high computational cost. First, the SNLCM is used as a prior model to generate a so-called training set, that is constituted of the QoI and associated control parameters. These control parameters belong to an admissible set, and are randomly drawn following a uniform distribution. Second, the target dataset is obtained through numerical simulations, using the SNLCM, where the elasticity matrix is taken as deterministic, as slightly stiffened with respect to the mean elasticity matrix. Also, the control parameters used for generating the target dataset belong to the same admissible set as for the training set, randomly drawn following a uniform distribution within cells of a regular grid. Once both the target dataset and the training dataset are obtained, the PLoM algorithm with constraint is used for obtaining a statistical surrogate model that is devoted to updating the statistical prediction of the QoI with respect to the control parameters. The PLoM algorithm generates a so-called learned dataset with same format as the training dataset, that takes into account the target subset of QoI. The learned dataset yields updated QoI as model outputs, which are updated with respect to the training dataset, so as to better match the target.

Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE SIMULATION OF SLOT DIE COATING USING DARCY-BRINKMAN-BIOT APPROACH

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ABSTRACT

The penetration of coating fluids in porous systems during single-layer slot die coating processes has been studied in various fields of manufacturing including fuel cells, photovoltaics and paper manufacturing. An adequate level of penetration is usually required during such a process to ensure proper adhesion of the coating fluid to the substrate. Insufficient or excessive penetration is undesirable because it can reduce the overall quality of the finish. Most computational studies carried out to study this phenomenon during the coating process generally adopt a decoupled approach due to the difficulty in coupling the pressure in the coating bead to the porous material. Attempts that have been made to study this concept within a fully coupled system, typically implement a visco-capillary model for the coating bead region and employ a 1D or 2D Darcy model for predicting the fluid penetration within the porous region. However, to fully understand the dynamics within the fluid domain, a 3D model fully coupled model is required. In this work, we employ the Darcy-Brinkman method to carry out the multiscale simulation of single-layer slot-die coating by introducing an extra drag term in the momentum equation that enables the direct coupling of flow in the coating bead to the flow in the porous material. This gives rise to a micro-continuum framework that solves for flow in the coating bead using the Navier-Stokes equation, while the flow in the porous medium is captured using the Darcy equation, thus creating a fully coupled system. This approach satisfies pressure and velocity continuity across the boundaries of both domains while still having distinct domains. Due to the porovisco-plastic nature of the coated substrate, our model also captures flow-induced material deformation such as wrinkling which can during this coating process. Such deformation is described by directly coupling the Darcy-Brinkman equation with the Biot equation for the deformed solid matrix. The model is then validated against single-layer slot die experiment with Carbon paper Toray 090 paper as the substrate, coated with a Newtonian bio-polymer fluid to accurately capture the depth of penetration in the deformable medium.

Uncertainty quantification and scientific machine learning for predictive modeling of complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADAPTIVE STRATEGIES FOR VALIDATING AND SELECTING PREDICTIVE PHYSICS-BASED AND MACHINE LEARNING SURROGATE MODELS

Danial Faghihi[*1], Pratyush Kumar Singh[1] and Kathryn Maupin[2]*

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ABSTRACT

This work presents two computational frameworks derived from the Occam-Plausibility ALgorithm (OPAL) for selecting an "optimal" predictive model from a multitude of potential physics-based and neural network surrogate models, each differing in fidelity and complexity. OPAL relies on the notation of prediction pyramid signifying the hierarchy of scenarios to systematically inform the model and leverages Bayesian inference for model calibration and validation and the notion of model plausibility to systematically select the simplest valid model that delivers sufficiently accurate computational prediction. The critical feature to ensure the model's predictive ability is the design of model-specific validation experiments to provide observational data reflecting, to some extent, the structure of the target prediction. The applications of these frameworks in multiscale modeling of microscale materials and neural network surrogate models of mesoporous building insulation components will be discussed.

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16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

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July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DISCOVERING OPTIMAL PREDICTIVE DEEP LEARNING SURROGATE MODELS USING THE OCCAM-PLAUSIBILITY ALGORITHM

Danial Faghihi[1], Pratyush Kumar Singh*[2] *and Kathryn Maupin*[3]

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ABSTRACT

This work introduces a novel framework, built on the Occam-Plausibility Algorithm (OPAL), for strategically discovering of "optimal" predictive neural network surrogate models for high-fidelity physical simulations. Leveraging hierarchical Bayesian inference to determine neural network parameters and hyper-parameters, along with Bayesian model validation principles for credibility assessment, the proposed OPAL-Surrogate systematically identifies the simplest credible (“optimal”) surrogate model capable of delivering accurate and reliable predictions. The proposed strategy embraces the concept of a prediction pyramid, representing a hierarchy of scenarios to inform the model systematically. A key aspect ensuring the model's predictive ability is the design of model-specific high-fidelity scenarios to provide training data reflecting the structure of the target prediction. The application of this framework in surrogate modeling includes multiscale simulations of mesoporous building insulation materials and turbulence combustion simulations, which will be discussed.

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Multi-scale, multi-rate damage and fracture: Models, experiments, and simulations
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CHARACTERIZATION AND MODELLING OF THE EFFECTS OF WEAVING DEFECTS ON THE MECHANICAL BEHAVIOUR OF L-ANGLE THERMOSET COMPOSITE SPECIMENS.

Christian Fagiano[1], Anton Koenig[1], Claire Fougerouse[1], Florence Saffar[1] and Frédéric Laurin[1]*

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ABSTRACT

Structural parts made of laminated composite materials with long carbon fibers are used today in a growing number of high-performance industrial applications. However, due to their manufacturing process, composite structures have different types of initial defects which can lead to a significant reduction in their mechanical properties. Regarding the scientific literature, the analysis of out-of-plane waviness effects within L-angle thermoset composite specimens has been approached both experimentally [1] and with numerical simulations [1,2]. These defects can induce significant reductions in their mechanical strength due to premature failure by delamination. These reductions depend on the characteristics of the waviness defects, i.e. their geometry (length, amplitude, etc.) and their position in the part. Predicting the reduction in mechanical properties is essential for defining acceptance and certification criteria for structural parts in presence of initial defects representative of those observed at industrial production sites.

The purpose of this work is to better understand the damage and failure scenarios of L-angle thermoset composite specimens subjected to four-point bending tests in presence of out-of-plane waviness defects. To do this, a numerical strategy for predicting these reductions, based on finite element simulations, has been implemented at ONERA. The geometry of the defect is explicitly considered in the mesh from microscopic or tomographic observations of the specimens tested. In order to validate the proposed numerical approach, an experimental campaign of multi-instrumented tests is carried out.

First, L-angles specimens with initial defects of industrial interest are manufactured. Then, mechanical characterization through heavily instrumented mechanical tests is performed. The experimental setup definition is assessed by preliminary simulations and 3D virtual modelling techniques. Finally, finite element simulations of the experimental tests are simulated using Zébulon (finite element solver of the Z-set suite) by means of parametrical models available at ONERA. The comparison between numerical simulations and experimental observations show a good agreement and allows a better understanding of the characteristic damage mechanisms.

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Probabilistic learning and constrained generative models for uncertainty quantification
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

UNSUPERVISED DISENTANGLEMENT AND DIMENSION REDUCTION FOR LARGE-SCALE ENGINEERING SYSTEMS

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ABSTRACT

Numerous scientific and engineering systems are inherently high-dimensional and multi-modal. We present GM-VAE, an unsupervised generative learning method that provides dimension reduction and clustering of complex, high-dimensional scientific data. The GM-VAE model comprises a variational autoencoder with a Gaussian mixture model in the latent space. During training, the model learns an evolving low-dimensional latent manifold of the data, facilitating disentanglement into clusters and yielding optimal dimension reduction and clustering. We propose a training strategy that combines the expectation maximization (EM) algorithm and gradient descent for improved accuracy. Through experiments with large-scale datasets from turbulent combustion systems, representations learned by the GM-VAE model provide a physically interpretable dimension reduction, enabling a better understanding of the high-volume, high-dimensional data from various sources. In addition, the GM-VAE framework facilitates comparisons between different physical mechanisms, modeling fidelities, and experiments against simulations.

CONSTITUTIVE MODELING AND NUMERICAL SIMULATION OF BIGHORN SHEEP HORN UNDER IMPACT LOADING

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ABSTRACT

Bighorn sheep (Ovis canadensis) is known for its giant spiral horns that can sustain impact loading at a speed up to 5.5 m/s during ramming without causing severe damage or head concussion. The horn of the bighorn sheep is composed of a keratin-based biological material with a tubule-lamella structure. This special structure gives the horn material anisotropic hardening characteristics under impact loading. Investigating the mechanisms of energy dissipation of bighorn sheep horn can inspire the design and development of new materials with high capacity of energy dissipation and/or impact mitigation.

In this study, a transversely isotropic constitutive model with anisotropic hardening and strain-rate effects was developed for predicting the mechanical responses of the horn under impact loading. The characterization of material properties was conducted using test data from uniaxial compression tests of the horns under both quasi-static and dynamic loading. The constitutive model was later implemented into the commercial finite element code, LS-Dyna, as a user-defined material subroutine and was validated against test data. The user-defined constitutive model was subsequently used in finite element simulations of dynamic impacts on the bighorn sheep horn to study the mechanical responses of the horn material subjected to large impact loads without causing severe damage. The mechanism of energy absorption and dissipation, stress distributions, and propagation of displacement waves was also investigated.

Numerical methods, mathematical modeling and analysis in material science
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEEPN^2: A MACHINE-LEARNING BASED NON-NEWTONIAN HYDRODYNAMIC MODEL WITH MOLECULAR FIDELITY

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ABSTRACT

A long-standing problem in the modeling of non-Newtonian hydrodynamics of polymeric flows is the availability of reliable and interpretable hydrodynamic models that faithfully encode the underlying micro-scale polymer dynamics. The main complication arises from the long polymer relaxation time, the complex molecular structure, and the heterogeneous interaction. We developed a deep learning-based non-Newtonian hydrodynamic model, DeePN^2, that enables us to systemically pass the micro-scale structural mechanics information to the macro-scale hydrodynamics for polymer suspensions. The model retains a multi-scaled nature with clear physical interpretation and strictly preserves the frame-indifference constraints. We show that DeePN^2 can faithfully capture the broadly overlooked viscoelastic differences arising from the specific molecular structural mechanics without human intervention.

Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SOME RECENT ADVANCES IN STRUCTURAL DAMAGE TRACKING AND MONITORING

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ABSTRACT

Damage tracking and monitoring from digital twins and in situ measurements, through the DDDAS framework, has been one of the numerous research topics addressed by J.T. Oden. In his memory, the talk will present some recent developments on this critical issue, which aim to design smart and autonomous mechanical structures able to perform online control of their health and take anticipated actions during service. An innovative cross-disciplinary approach will thus be presented, which performs fast sequential data assimilation from hybrid twins. This approach couples several advanced numerical methods such as model reduction, adaptive modeling, or Kalman filtering, together with a specific cost function which brings robustness faced to highly nonlinear models, various uncertainty sources, and real-time computation constraints. Its capabilities will be shown on several practical engineering applications when inferring real data on-the-fly and performing online health monitoring on large scale structures.

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M. Diaz, P-E. Charbonnel, L. Chamoin, Fully automated model updating framework for damage detection based on the modified Constitutive Relation Error, Computational Mechanics, online, 2023

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Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HYDROMECHANICAL CONSTITUTIVE TENSOR AND INSTABILITY ANALYSIS OF PARTIALLY SATURATED GEOMATERIALS VIA A DISCRETE ELEMENT APPROACH

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ABSTRACT

The current research employs a micromechanical approach to characterize the hydromechanical behavior of partially saturated geomaterials within the pendular saturation regime. Using Discrete Element Method (DEM) modeling, this study focuses on elucidating the hydromechanical constitutive relationship and instability of densely packed granular materials under triphasic (solid, water, and air) conditions involving isolated liquid bridges.

Within the elastoplasticity framework, a new numerical scheme is proposed to derive a general hydromechanical constitutive tensor (tangent operator) considering the appropriate stress and strain conjugates. The incremental tangent operator is numerically reconstructed through a complete multi-directional DEM probing at various reference material states. The computed constitutive tensor can be integrated into a bifurcation analysis by evaluating its spectral characteristics.

The second-order work instability criterion is evaluated through DEM simulations by applying perturbations near the stress limit state of a deviatoric loading path. In a partially saturated state, defining the second-order work instability criterion is involved due to the interplay between stress and strain variables, influenced by coupled hydromechanical effects [1]. The multiphysics and multiphasic interactions arising from the capillary effect at the microscale result in intricate macroscale behaviors under triphasic conditions. In this regard, the external and internal second-order works are evaluated using DEM to capture the instability with respect to stress-strain variables in wet conditions. Consistent with the spectral analysis of the computed constitutive tensor, and the vanishing of its mechanical part, the second-order work results support the ‘effective’ role of contact stress in describing failure in wet granular materials.

Finally, a mesoscale analysis is presented to detect shear band localization and validate the well-known Rice criterion [2] within a micromechanical framework. The DEM sample is divided into mesoscale cells, each regarded as a representative elementary volume, allowing the correlation of mesoscale stress and strain through a constitutive law. The presented methodology, which incorporates the use of the tangent operator in the acoustic tensor, interestingly reveals that Rice’s localization criterion reasonably detects the orientation of shear bands when applied to the mechanical part of the hydromechanical tangent operator.

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SciML in the real world
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMPROVING THE ACCURACY AND SCALABILITY OF LARGE-SCALE PHYSICS-BASED DATA-DRIVEN REDUCED MODELING VIA DOMAIN DECOMPOSITION

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ABSTRACT

This presentation focuses on the construction of accurate and scalable data-driven reduced models of large-scale simulations with complex dynamics and sparse training data sets. In these settings, standard, single-domain approaches may be too inaccurate or may overfit and hence generalize poorly. Moreover, the memory and computing resources to train such models can be prohibitive in practice. To address these challenges, we introduce a domain decomposition formulation into the construction of a data-driven reduced model. In doing so, the basis used in the reduced model approximation become localized in space, which can increase the accuracy of the domain-decomposed approximation of the complex dynamics. The decomposition furthermore reduces the memory and computing requirements to process the large-scale training data set. We demonstrate the effectiveness and scalability of our approach in a large-scale three-dimensional unsteady rotating detonation rocket engine simulation scenario with over 75 million degrees of freedom and a sparse training data set. Our results show that compared to the single-domain approach, the domain-decomposed version reduces both the training and prediction errors for pressure by up to 13% and up to 5% for other key quantities, such as temperature and fuel and oxidizer mass fractions. Lastly, our approach decreases the memory requirements for processing by almost a factor of four, which in turn reduces the computing requirements as well.

Predictive digital twins
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NONPARAMETRIC PROBABILISTIC FRAMEWORK FOR DIGITAL TWINNING

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ABSTRACT

A digital twin (DT) usually refers to a digital replica of an asset that can be used, for example, to optimize in near real-time the operation and/or life cycle management of the asset; or more generally, to drive the Intelligent Enterprise by linking engineering and operations such as maintenance. The enabler often advocated for such a technology is the integration of artificial intelligence, machine learning, and software analytics with data, to create living digital simulation models capable of updating themselves as their physical counterparts evolve. Preliminary forms of such DTs are often presented as the result of a synergy between data analytics and the model-based prediction of a few, scalar, quantities of interest (QoIs). This lecture however will question whether a few QoIs can always be identified to represent the critical state of a newly designed then deployed physical platform. It will argue that whereas Digital is the relatively easy part of a DT that everyone talks about, Twin is the more difficult part that few are working on. Yet, the biggest concern that most stakeholders have is the risk of misrepresenting the physical asset they want to replicate using a DT. To this end, the lecture will present a more robust approach for realizing DTs based on adaptable, stochastic, low-order but high-fidelity computational models grounded in physics. The proposed approach features novel mathematical ideas for integrating the modeling and quantification of model-form uncertainty with probabilistic reasoning, projection-based model order reduction, and machine learning. It constructs stochastic, physics-based computational models that self-adapt using information extracted from sensor data; and operate in real time or near-real-time. Finally, the lecture will demonstrate the potential of the proposed approach for digital twinning using several realizations, including: a DT of a small-scale replica of an X-56 type aircraft for ground vibrations assessment; a DT of the front bumper of a 2013 Honda Accord EX-L for crash prediction and analysis; and a DT for the structural health monitoring of an aircraft wing.

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Computational mechanics of soft matter and machines
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HYPERELASTICS.JL: THE LARGEST COLLECTION OF HYPERELASTIC MODELS FOR SOFT MATERIAL MODELING AND SIMULATION

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ABSTRACT

For soft matter simulations in various applications, an appropriate selection of the hyperelastic material model is necessary for accurate prediction and calibration. In most commercial codes, a limited number of hyperelastic models have been implemented, which limits applications in various fields such as biomimicry, medical, etc. We have developed and deployed Hyperelastics.jl, a Julia language-based library that contains the largest set of implemented hyperelastic models to date. Within Hyperelastics.jl, over 70 compressible and incompressible models have been implemented for automatic differentiation. The use of automatic differentiation within the package limits the barrier to entry for developing new material models by requiring only a form for the strain energy density function. The package provides the most common analytical methods and extensions of models for compressible materials. Further, the package provides some data-driven methods for prediction. By using the Julia language, the models are readily compatible with FEA methods from Gridap.jl and Ferrite.jl. Further, the package includes extensions for material model calibration from multiple uniaxial and biaxial tests with customizable loss functions. The simplicity of the package aims to decrease the barrier for implementing and testing less common hyperelastic models for soft matter simulations. Future works will aim at expanding to the modeling of other non-linear—such as viscoelastic, other mechanical, electro-mechanical, and opto-mechanical—mechanisms with the goal of developing a more complete soft material modeling suite.

Industrial applications of IGA
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A COMPARATIVE STUDY OF C0, C1, AND G1 SPLINE CONSTRUCTIONS AROUND EXTRAORDINARY POINTS

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ABSTRACT

Extraordinary points (EPs) are required to represent manifold surfaces with arbitrary topological genus. G-splines are a generalization of B-splines that deal with extraordinary points by imposing G1 constraints across their spoke edges. As explained in [1], G-splines combine the following distinctive characteristics: (1) Only vertex-based control points are used and they behave as geometric shape handles, (2) any control point of the control net can potentially be an EP, (3) global C1 continuity in physical space is obtained without introducing singularities, (4) faces around EPs are not split into multiple elements, i.e., meshes with uniform element sizes are obtained, and (5) good surface quality is attained. After comparing the spectral accuracy when solving eigenvalue problems, the accuracy in L2 and H1 norms when solving linear elliptic problems, and the surface quality, we conclude that G-splines are more suitable for IGA than EP constructions based on the D-patch framework [2, 3].

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Physics-informed machine learning for numerical modelling in engineering and science
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INTEGRATING PHYSICS-INFORMED NEURAL NETWORKS AND COMPUTATIONAL FLUID DYNAMICS TO OPTIMIZE BAKING OVEN PERFORMANCE

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ABSTRACT

This study introduces an innovative method to enhance the precision of simulations for baking ovens by merging traditional Computational Fluid Dynamics (CFD) techniques with Physics-Informed Neural Networks (PINNs). Our effort is concentrated on creating a detailed representation of airflow and heat distribution within a commercial baking oven by integrating fan modeling techniques into the turbulent, unsteady simulation of the baking chamber. This integration effectively captures the fan's influence on the oven's airflow patterns and temperature distribution.

Utilizing Moving Reference Frame (MRF) data provides a deeper insight into the fan's effect on the oven's internal environment, leading to enhanced simulation outcomes. However, this method in unsteady simulation introduces a limitation due to the fan geometry being fixed in the global reference frame, resulting in non-physical low-velocity regions in the wake of the blades. Although the Sliding Mesh (SM) approach offers greater accuracy by utilizing an unsteady solver, it demands higher computational resources. By training the PINNs with fan data through MRF and SM, we simulate the fan with its actual geometry at different rotation speeds quickly and accurately. We achieved airflow and temperature profile with accuracy comparable to conventional CFD methods but with reduced computational costs across various operating conditions. Incorporating PINNs into CFD simulations that are used for the whole oven simulation not only boosts efficiency and accuracy but also addresses the limitations of traditional CFD models, particularly in the high computational cost of capturing transient behaviors and complex flow phenomena. This signifies that our PINN-CFD methodology holds significant promise for designing and optimizing ovens, potentially elevating their functionality. Furthermore, it paves the way for employing machine learning techniques in thermal and fluid flow engineering, an invaluable asset in situations where computational resources are scarce or swift simulations are essential without sacrificing precision.

Multi-scale modeling and upscaling for flow induced vibrations, from local reference simulations to certified industrial tools
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TIME-STEPPING STRATEGIES FOR NON-LINEAR MULTI-SCALE FLUID-STRUCTURE DYNAMICS WITH PARTITIONED COUPLING

Vincent Faucher[*1] and Maria Adela Puscas*[1]

[1]*CEA*

ABSTRACT

The present contribution is dedicated to providing some review, insights and recent advances in the field of time algorithms for fluid-structure dynamics with non-linear structural behaviour solved within a partitioned coupling between specific software. The structural non-linearities can be related to internal behavior, contact/impact and/or rupture and fragmentation, implying the resort to explicit time integration for the sake of robustness of the structure solver. Such a choice naturally introduces time-multiscale problematics in the coupled problem, since fast waves setting the critical time step in the structure are likely to generate a significantly more restrictive stability constraint than for the fluid, which on the other hand is likely to concentrate most of the computational effort.

Several configurations shall be considered to provide significant results for the community. First, the most classical situation of compressible transients with explicit time integration for both fluid and structure will set the bases of the multi-scale time stepping with various sound velocity for fluid and structure. Second, the compressible fluid solver will be replaced by an incompressible CFD solver, for a different range of transients in the vibratory dynamics and flow induced vibrations regime. Here, the question of Arbitrary Lagrangian Eulerian approaches for the fluid shall be particularly considered, with specific time scale possibly introduced by the management of the arbitrary fluid grid motion itself. Finally, the last configuration will add contact and impacts to the fluid-structure problem, introducing the complementary need for adaptive subcycling strategies following the thorough monitoring of impact history, to provide both computational efficiency and accuracy in terms of fluid response to severe discontinuities in the structural forces.

Examples will be provided in the field of safety and performance for nuclear pressurized water reactors. Some past references are provided for illustrative purposes.

Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CRITICAL PLANES ANALYSIS OF THE IMPACT OF POROSITIES ON THE FATIGUE OF METAL SOLIDS

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ABSTRACT

In this work, we take interest to the impact of defects present in metal solids manufactured by material fusion or by additive manufacturing on their fatigue life during cycling loading. Indeed, we observe a more or less strong local plasticity around the defects even if the stresses remain below the elastic limit, which can strongly impact the fatigue life of such solids. In the case of a part obtained by steel casting, it is the retassures that make the part most vulnerable. In the case of solids obtained by additive manufacturing, the most damaging defects are surface roughness and porosities linked to a lack of fusion. In order to estimate the fatigue life of such solids, it is necessary to observe the states of stress and deformation around the defects during a cycle. As stress levels can be relatively high locally, critical plane type criteria are relevant for estimating the fatigue life of such solids. In order to carry out a fatigue analysis of a part obtained by steel casting or by additive manufacturing, we propose to model it by finite elements, with a refinement of the elements around the porosities, then to calculate the local stress and deformation states, and finally to implement a critical plan type criterion, like the Fatemi-Socie criterion. The critical planes are the planes on which the maximal shear deformation amplitudes occur. The local stress and strain states can be highly multi-axial. So the determination of the critical planes can be very computationally and storage consuming. In the present work, an analysis in the space of deviators of the deformation tensor makes possible determination of such planes in each of the numerous nodes of the mesh[1]. These three steps of calculation, correlated with experimental tests, makes it possible to envisage obtaining fatigue life laws for numerous metallic materials presenting defects.

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Current trends in phase-field modeling and computations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EMERGING ANISOTROPY AND TETHERING WITH MEMORY EFFECTS IN FIBROUS MATERIALS

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ABSTRACT

Fibrous materials may undergo an internal reorganization, which turns out in the emergence of preferential directions. This is a peculiar behavior of many biological tissues, which drive reorientation by external stimuli at chemo-mechanical levels. In particular, it is detected that contractile cells can reorganize fibrous extracellular matrices and form dense tracts of aligned fibers (tethers), that guide the development of tubular tissue structures and may provide paths for the invasion of cancer cells. Tether formation is caused by buckling instability of network fibres under cell-induced compression. We present a simple phase-fiel model that captures the essential aspects of these phenomena. The model qualitatively describes: (i) the emergence, induced by local compressive strain, of anisotropy, where fibrous materials exhibit directional preferences; (ii) the occurrence of micro-buckling, which leaves a lasting plastic deformation in the material; and (iii) the formation of localized field patterns, which contribute to the overall behavior of the material.

HYPERBOLIC MODELING OF GRADIENT DAMAGE AND ONE-DIMENSIONAL FINITE VOLUME SIMULATIONS

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ABSTRACT

This study [1] provides a new formulation of gradient damage model which allows an efficient explicit numerical solution of dynamics problems. The proposed methodology is based on an "extended Lagrangian approach" developed in [2] for the nondissipative and dispersive shallow water equation. By using this strategy, the global minimization problem commonly derived for gradient damage models is recast as a purely local hyperbolic one with source terms that can be easily solved using finite volumes. The numerical solution of the governing system is then based on a fractional-step method consisting of a classical Godunov-type scheme and an implicit Ordinary Differential Equation solver for the local source terms. Numerical results are presented on the one-dimensional multi-fragmentation and spalling tests for illustration purpose.

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Enabling technologies for digital twins: Model reduction and scientific machine learning
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MODULARIZED WORKFLOW FOR SURROGATE MODELING OF TURBIDITY CURRENTS

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ABSTRACT

Turbidity currents are major agents of sediment transport in land and aquatic environments. They are important for their potential environmental hazards and volume share on the deep sea's clastic accumulations [1]. Turbidity flows are formed when the density difference between sediments and fluids generates a driving force that induces fluid motion. Numerical simulations considering the discretization of the governing Partial Differential Equations (PDEs) usually offer detailed insights with the cost of being computationally expensive, given the complex nature of the physics of the problem. This study focuses on developing a modular workflow that creates surrogate models for turbidity currents to replace costly simulations with more efficient data-driven alternatives. The workflow orchestrates steps such as data ingestion, data normalization, linear and nonlinear dimensionality reduction, data splitting, and the Scientific Machine Learning (SciML) model for training and inference and data post-processing. Having a computational workflow that is able to generate multiple surrogate model configurations allows faster experimentation and model selection for better predictions. Here, we employ stabilized finite elements to generate the training data for surrogate modeling. Two distinct applications for surrogate models are explored: temporal predictions for estimating future flow and extrapolation of simulated parameters for further exploration. We test the behavior of different SciML techniques to address the two aspects of surrogate modeling mentioned above. The list includes Dynamic Mode Decomposition [2], Gaussian Processes, and Neural Networks [3]. The study's applications are tested using the lock-exchange configurations, incorporating various physical aspects such as deposition and erosion, allowing a more comprehensive evaluation of the surrogate models' performance under diverse conditions. Preliminary results showcase the effectiveness of the surrogate models in accurately predicting turbidity currents. The temporal prediction approach demonstrates its potential for forecasting future flow conditions, while the parameter extrapolation approach extends the applicability of the models beyond the simulated scenarios.

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Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

QUASI-DYNAMIC PHASE-FIELD MODELING OF IN-PLANE DEFORMATION AND GROWTH OF GEOLOGIC FAULTS

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ABSTRACT

Earthquakes are typically triggered by the dynamic deformation and growth of geologic faults which are discontinuities or narrow zones within the Earth's crust. During and after the earthquake process, a fault system commonly exhibits a variety of geometric features (e.g., fault kinking and branching) due to structural and material complexities. These intricate geometric features, however, pose a substantial challenge to existing fault rupture models that treat the fault as a lower-dimensional manifold in a continuous domain. To overcome this challenge, a phase-field model has recently been developed to simulate quasi-dynamic sliding and growth of rate- and state-dependent frictional faults [1]. Nevertheless, this preliminary work restricted its focus to a 2D anti-plane condition, while the fault system under an in-plane or more general 3D condition manifests more realistic and complex structural properties (e.g. en enchelon faults). In this work, we extend the previous anti-plane model to an in-plane version by incorporating additional kinematics and pressure-dependent shear strength. Numerical simulation of a benchmark example verifies that the extended phase-field model can accurately capture the quasi-dynamic, rate- and state-dependent frictional behavior in an in-plane setting. Additional simulations involving fault nucleation and propagation under in-plane boundary conditions further demonstrate the capability of the phase-field model to handle arbitrary geometric features emanating from structural complexities and material heterogeneities. This phase-field model enables more efficient and realistic modeling of fault systems, with potential to improve the understanding of seismic source mechanics and consequently advance the next-generation seismic hazard models.

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Lattice Boltzmann modelling and study of complex flows
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LARGE SCALE DIRECT NUMERICAL SIMULATIONS OF FORCED CONVECTIVE BOILING

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ABSTRACT

Advancing our understanding of forced boiling convection is essential for optimizing heat transfer and energy efficiency in various industrial processes. While general insights into boiling phenomena exist for pool boiling systems, where the vapor bubbles and heated liquid are influenced solely by gravity, forced boiling has received much less attention, with few recent preliminary works reporting results from 2D simulations [1,2].

In this work, we present results of fully 3D numerical simulations of forced boiling convection. We leverage on a highly optimized cascaded lattice Boltzmann method (LBM) code [3] based on the Multi-GPU accelerated computations by the hybrid OpenACC and MPI approach, allowing for an extensive parameter scan to analyse the impact of external forcing on the boiling curve, depicting the relationship between heat flux and wall superheat. We show that within an optimized parameter range, the window of nucleate boiling for highly efficient heat transfer is extended while mitigating the risk of transition to film boiling.

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Certification of simulations and model adaptation in computational science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADAPTIVE APPROXIMATION OF STOCHASTIC PROCESSES

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ABSTRACT

There are many stochastic processes which are known to be arbitrarily hard to approximate when using uniform timesteps.
This can even happen if the coefficients (drift and diffusion) of the governing stochastic differential equation are smooth. Practically more relevant is for
example the Cox-Ingersoll-Ross process, which has a square root singularity in the diffusion term. It is known that uniform approximations of the process converge
with arbitrarily small algebraic rate. We demonstrate numerically, that adaptive mesh refinement in time can overcome this barrier and deliver the expected convergence rates
of 1/2. This is particularily interesting since multi-level approximations require exactly this rate to offer a significant performance gain.

ERROR ESTIMATION FOR REDUCED-ORDER MODELING OF PARAMETRIC NONLINEAR DYNAMICAL SYSTEMS

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ABSTRACT

Model order reduction (MOR) for parametric dynamical systems has been an active research topic for many years. We present two new contributions to this topic: 1) accurate error estimation for reduced-order models (ROMs) solved with any black-box time-integration solver. 2) Inf-sup-constant-free output error estimation for ROMs of parametric dynamical systems. Accurate error estimation plays an essential role in constructing ROMs with reliable accuracy. For most of the existing a posteriori error estimation approaches, e.g., the residual-based error estimators proposed for the reduced basis method, details of the time integration scheme must be accessible. This poses a challenge when libraries with automatic ordinary differential equation integrators are used to solve the original dynamical systems and/or the corresponding ROMs. To address this issue, we present a data-enhanced approach [1] for a posteriori error estimation. This new approach enables residual-based error estimators to be independent of any time integration method. To this end, we introduce a data-driven closure term to a user-defined time-integration scheme. The closure-term aided error estimator can accurately estimate the error of the target ROM that can then be solved by any time integration solver. We use radial-basis function interpolation to accurately learn the closure term, using only a modest amount of training data. The new error estimator is incorporated within a greedy process to obtain parametric reduced-order models. Existing techniques of error estimation for time-evolution systems entail computing the parameter-dependent smallest singular values of a large matrix with the original system dimension. This is not only time-consuming for large-scale systems, but also makes the error estimation rough for problems with smallest singular values being close to zero. The smallest singular values are the so-called inf-sup constants. We propose an inf-sup-constant-free output error estimation [2] for time-evolution systems. Numerical tests on several engineering problems justify our theoretical analysis, showing that the proposed error estimation techniques outperform other existing error estimators.

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New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A ROBUST TOPOLOGY OPTIMIZATION FRAMEWORK UNDER MULTIPLE UNCERTAINTIES AND LARGE DEFORMATIONS

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ABSTRACT

In real-world applications, uncertainties in load, material, and geometric properties are present that should be addressed in a design process. To this end, a computational topology optimization framework is proposed for designing robust structures that are insensitive to the target stochastic variations in load, material, and geometric properties. In the proposed framework, various uncertain sources are modeled by random vectors or random fields. With good computational efficiency and accuracy, a stochastic perturbation approach is adopted within a stochastic finite-element-based method to compute statistical moments of structural end compliance under large deformations. The excessive mesh distortion issue under large deformations is addressed by leveraging an adaptive linear energy interpolation scheme based on modifications in free energy. In addition, the design sensitivities are computed by utilizing a consistent analytical adjoint analysis approach that is used in a gradient-based optimization formulation. Verification is performed both for the implementation of the uncertainty quantification and sensitivity analysis methods. Numerical results show that the response of robust designs is less sensitive to the variations of target uncertainties compared to their deterministic counterparts. Moreover, even without enforcing stability constraints, the robust optimization formulation may help to achieve a stable design whereas the deterministic design is unstable.

Buckling analysis and design of thin-walled structures based on novel and intelligent computational methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A GAUSSIAN PROCESS-DRIVEN WORST REALISTIC IMPERFECTION METHOD FOR BUCKLING ANALYSIS OF CYLINDRICAL SHELLS

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ABSTRACT

Thin shells are very efficient structures that can support very high buckling loads and hence their buckling and post-buckling behaviors have presented scientific and engineering challenges for decades. Extensive theoretical studies connect initial post-buckling behavior with imperfection sensitivity. It is necessary to accurately analyze the capability before optimizing the structure. However, the significant discrepancy in loading capability between the theoretical and experimental results severely limits the design of the structure.

We propose a Gaussian process-driven worst imperfection method to generate simulated geometric imperfections and find the lower limit of buckling capability. First, we utilize the nested stochastic Kriging to estimate the global trend and envelopes of the geometric imperfections. Second, the expansion optimal linear estimation and direct weighting construction method are used to expand limited data, which allows the simulated geometric imperfections to have the same characteristics as the initial data. Third, two magnitude-based constraints are provided, which can make the simulated geometric imperfections more consistent with the realistic data and can represent more design space. Finally, for the cylindrical shells, the data pre-processing method is further provided in this paper. Two numerical examples with assumed geometric imperfections are used to validate the proposed method, and the minimum buckling capacity of a cylindrical shell with 8 realistic geometric imperfections data is estimated. The results show that the proposed method can achieve the best performance in terms of accuracy, efficiency, and robustness.

A DATA-DRIVEN OPTIMIZATION FRAMEWORK FOR A HIGH-ORDER HYBRID SCHEME TOWARDS IMPLICIT LARGE EDDY SIMULATIONS OF COMPRESSIBLE FLOW

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ABSTRACT

Simulating compressible turbulent flows entails dealing with a broad range of genuine (e.g. shocks, high gradients) as well as non-genuine (e.g. turbulence) subgrid-scales and their intricate interactions. The challenge lies in developing a numerical scheme that physically consistently recovers or models such widely varying flow features, and ensures numerical stability, computational efficiency as well as generalization robustness, simultaneously. A hybrid scheme has been demonstrated to be an effective method towards simulating compressible flows with turbulent structures [1,2]. The scheme employs sensors to adaptively choose from different high-order numerical schemes, each fit to optimally address specific flow characteristics. However, the existing method of parameter fitting relies on expert insight, spectral analysis, or partial numerical experiments, which may not fully account for the complex nonlinear interactions among the whole scales during simulation. In this study, we present an innovative data-driven multi-objective optimization method for designing a hybrid scheme suited for implicit large eddy simulation of complex compressible flows. The scheme is optimized to achieve a balance between three objectives: limited numerical dispersion, realistic scale dynamics and kinetic energy conservation. We employ a multi-objective Bayesian optimization framework with an expected hypervolume improvement acquisition function to perform the optimization as proposed in [3]. The results demonstrate that the scheme converges to an optimal solution with only a very limited number of evaluations. The proposed hybrid scheme is validated on basis of flow configurations involving a wide range of characteristic single- and two-phase flow characteristics. The hybrid scheme is benchmarked to established higher order non-linear schemes, clearly indicating the superior performance of the high-order hybrid scheme for LES of compressible flows.

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Verification techniques in computational physics and applied mathematics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOWARDS HIERARCHICAL VERIFICATION BY UTILIZING SYMMETRIES

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ABSTRACT

Verification & Validation represents a portion of testing and strengthening the credibility of codes and establishing a sense of the numerical uncertainty of simulations. Verification focuses on mathematical accuracy, and typically leaves comparison with experiments to validation. Extending verification results towards simulations that analysts and experimentalists care about requires losing analytical rigor but gaining relevance. In this presentation we discuss anchoring complex but relevant simulations to simpler ones whose accuracy is easier to test. To do this we rely on the tight coupling between known solutions and their related symmetries. As we move away from analytic solutions, using the solution's symmetry as a guide, we move toward complex simulations of interest to analysts. Simultaneously, this should help the analyst see that if a code doesn't perform well on certain simpler tests then simulation results of interest should be analyzed cautiously.

Analysing complicated simulations often pushes analysts outside the realm where their intuition has been developed and may be reliable. This requires significant trust in a code's accuracy across many physics disciplines. Understanding the numerical space over which rigorous analytic solutions for testing codes exists is important for supporting trust-worthy assessments. Analytic solutions in any dimension or geometry rely on symmetries. Symmetries over manifolds are the subject of Lie groups. Numerical methods involving Lie group have recently been developed, called Lie Group Integrators, and promise to improve numerical methods along symmetries of a numerical manifold.

At a more fundamental level to code verification, little attention has been given to understanding where test solutions come from, and what different tests should tell code developers and code users. Different tests typically evolve along different orbits of a symmetry. Comparing code results against different analytic solutions thus says something about a code's performance along specifics orbits. Understanding the space of orbits and how a code performs near each should be helpful to understanding how a code performs away from those orbits. Of course, analyst's complicated simulations are not bound to a specific orbit, but it is hoped that understanding the numerical uncertainty of a code in the space between orbits will better help analysts understand the numerical uncertainty in their results.

Advanced numerical methods for complex flows and engineering challenges
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL STUDY OF THE BUBBLE RISING IN ELASTOVISCOPLASTIC FLUIDS USING THE GEOMETRIC VOLUME OF FLUID ALGORITHM

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ABSTRACT

This investigation delves into the dynamics of air bubble motion within liquids, a phenomenon of paramount significance in diverse domains such as heat transfer and material quality. Our endeavor entails the formulation of an innovative interface capturing technique tailored for simulating multiphase viscoelastic fluid flows. The algorithm we propose leverages a geometric volume of fluid methodology known as isoAdvector, steering away from conventional reliance on volume fraction gradients by incorporating a reconstructed distance function (RDF) to precisely ascertain interface curvature.

To fortify the precision and robustness of our approach, a piecewise linear interface construction (PLIC) scheme is integrated with RDF-based interface reconstruction. The culmination of these efforts is the development of the Multiphase Viscoelastic PLIC-RDF isoAdvector (MVP-RIA) algorithm. Numerical validation involved simulations of the buoyancy-driven rise of a bubble in an elastoviscoplastic liquid characterized by the Saramito-Herschel-Bulkley constitutive equation.

Our observations unveil a nuanced interplay of forces within very small air bubbles in elastoviscoplastic fluid, where the dominance of elasticity and capillary forces constrains bubble deformation. As the bubble volume expands, lateral stretching assumes a more pronounced role, culminating in the emergence of distinctive bifurcated tails. Ultimately, the bubbles adopt highly elongated shapes with sharper tails.

MECHANOBIOLOGY OF BONE ADAPTATION IN BAREFOOT RUNNING

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ABSTRACT

INTRODUCTION
Computational bone remodelling has been explored in many human activities, yet there are few examples of its application in the foot, which is a key joint that interacts the most with our environment primarily through gait. In this study we present the extension of a continuum level bone remodelling algorithm to include the ‘Mechanostat’, and its importance on realistic bone adaptation and numerical convergence. We present the model in the application of foot bone adaptation in barefoot runners. Bone density and trabecular architecture formation are contrasted with CT evidence to evaluate the model.

METHODS
A finite element foot model was developed from MRI scans. The model was segmented in the software Mimics, meshed in Hypermesh, and solved using Abaqus. Plantar fascia was represented by linearly elastic connectors whose stiffness was 200N/mm. The bones were modelled as linearly elastic isotropic materials with Young’s Modulus of 7300MPa and Poisson’s Ratio of 0.3, and the lumped soft tissue surrounding the bone was a linear elastic model with Young’s modulus of 0.15MPa and Poisson’s ratio of 0.45 [1]. OpenSIM was used to compute the Achilles tendon force. Plantar pressure measured during gait and Achilles tendon force were applied to load the foot. A continuum damage mechanics model [2] with an ability to evolve the setpoint value following the cellular accommodation theory [3] was employed to predict the osteogenic responses. An adult model was customised to temporal hopping data and then used to predict heel bone adaptation of a change in running strike pattern from classical rearfoot to forefoot running. The Abaqus model predicted the bone density and structural changes in the heel bone (calcaneus).

RESULTS AND DISCUSSION
The model predicted the formation of a cortical bone layer like that observed in adult CT and predicted future temporal bone density consistent with measured DEXA scans. The model predicted higher heel bone density in forefoot strike runners despite the heel not actually touching the ground during running. This is likely due to higher Achilles tendon force and is consistent with measurements in the running literature. The ‘Mechanostat’ adaptation improved convergence of the model and ensured that the bone reached a saturation point and did not continue to adapt unconstrained.

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Multiscale computational and data-driven approach of advanced materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MATRIX ANALYSIS OF MOLECULAR STRUCTURES: FROM LINEAR ANALYSIS TO BUCKLING

Andrés Fernández San Miguel[1], Iván Couceiro Aguiar*[1], Luis Ramírez[1] and Fermín Navarrina Martínez[1]*

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ABSTRACT

One of the great successes in the field of engineering, whether aeronautical, civil, or mechanical, was the development of the Finite Element Method, thanks to which problems of solid mechanics, fluids and even fluid-structure interaction can be solved with great precision. In its origins, the method was applied mainly to macroscale problems, while at the atomic scale the use of Molecular Dynamics has been the more usual way.

As an alternative to the Molecular Dynamics method, we propose a new formulation that allows obtaining the stiffness matrices directly from the force-field, without resorting to simplifications other than those used in its parameterization. The formulation allows both first order analysis, linear instability, and geometric nonlinear analysis.

In the case of first-order analysis, we applied this formulation to the vibrational analysis of different simple molecules [1,2], also including the parameterization of its force constants [2]. In turn, it has been applied to the study of the mechanical behavior of protein structures, such as coronavirus spikes or viral capsids.

The formulation has also allowed the study of linear buckling of structures such as carbon nanotubes and graphene sheets, allowing the development of equivalent continuous models of increasing interest in materials science [3]. Moreover, the inclusion of geometrical nonlinearities has allowed the study of nonlinear phenomena such as buckling in nanotubes both as monolayer and multilayer or in fullerenes.

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Emerging topology and shape optimization techniques in computational design of materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION OF TRUSSES AND FRAMES ACCOUNTING FOR STABILITY AND INITIAL POST-BUCKLING RESPONSE

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ABSTRACT

Sizing and topology optimization (TO) with maximum stiffness or stress reduction objectives often leads to designs that are highly sensitive to imperfections, and prone to geometric instabilities. Therefore, recent works have focused on introducing stability constraints, or on optimizing some nonlinear response functions, such as complementary work, end compliance, etc., achieving important results both in terms of computational efficiency and design novelty [1,2].

However, stability constraints only increase the initial buckling strength of the design, without giving any control neither on its imperfection sensitivity, nor on its actual buckling mechanism. Also, the optimization of non-linear response functions is almost always limited to the pre-buckling regime. To control the buckling mechanism, the post-buckling behavior must be investigated, and this requires computationally expensive path-following procedures which are often complicated by the interaction of nearly simultaneous buckling modes, frequently occurring for optimized designs.

An appealing alternative is offered by the asymptotic post-buckling (APB) theory [3], which provides an accurate approximation of the nonlinear response, close to a buckling point. Requiring one eigenvalue buckling analysis, and a few linear analyses, APB is a cheap computational tool for post-buckling simulation but is seldomly used for optimal design [4], and essentially missing in TO.
In this talk we apply APB theory to the optimization of the initial post-buckling behavior of trusses and frames. We consider compliance minimization problems, with constraints on the initial post-buckling coefficients, to ensure the systems' post-buckling stability. We also show how the APB theory can be used to generate an approximation of some non-linear response functions in the post-buckling regime. Basing the discussion on these simple structural models, we will review the points of cautions one needs to consider in the finite element implementation, discussing the suitability of the approach to large-scale problems, and more advanced continuum modelling.

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FAST PREDICTION OF CLUSTER INTERACTION TENSORS THROUGH DATA-DRIVEN SURROGATE MODELING

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ABSTRACT

One of the pressing challenges in computational solid mechanics is performing fast mechanical simulations of the multiple length scales of materials. Accomplishing this goal is essential to perform feasible multi-scale coupled analyses of materials and generate large material (synthetic) datasets required to train data-driven surrogate models [1].

In this context, Liu and coworkers [2] proposed the Self-consistent Clustering Analysis (SCA), a reduced-order method that achieves a striking balance between accuracy and efficiency. The core idea of the model reduction lies on a clustering-based domain decomposition performed in a preliminary offline-stage (learning). Similar to mesh-based simulations, the solution precision and computational cost depend on the number of clusters. As expected, the computation cost of the so-called Cluster Interaction Tensors (CITs) increases significantly with the number of clusters, thus raising a bottleneck in the learning process. In addition, such tensors are also recomputed during the online-stage (prediction) in the recently proposed extension called Adaptive Self-consistent Clustering Analysis (ASCA) [3], which further stresses the need of speeding up their computation.

In this contribution, we take advantage of a data-driven surrogate modeling approach to predict CITs directly from the clusters support functions. Deemed as key aspects, the efficient generation of a large representative training dataset and the choice of a suitable model architecture are discussed. Several comparisons between the predictions and the complete computation of the CITs demonstrate the performance of the data-driven model in terms of accuracy and computational time. Finally, the efficacy of the new approach is assessed in the multi-scale analysis of heterogeneous materials.

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Multi-scale, multi-rate damage and fracture: Models, experiments, and simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HOMOGENIZATION STRATEGY FOR THE PHASE-FIELD MODEL FOR PRESSURIZED FRACTURES

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ABSTRACT

Phase field model (PFM) for fracture is a relatively recent study and it has already been proven to be a propitious approach for modeling complex fractures. The PFM, based on a variational formulation, is able to automatically identifying multiple crack emerging and propagation, as well as representing bifurcation, nucleation and branching phenomena. For these reasons, the classic formulation has been extended to represent a variety of multiphysics problems, including hydraulic fracturing. Most hydraulic fracturing applications deal with materials that are heterogeneous at a certain scale. Adding the heterogeneous nature of the materials with the great difference of scales involved in the global problem make the study of hydraulic fracture from a multiscale approach an interesting topic to be explored. However, there are few proposals in the literature for applications of the PFM for fracture in the context of a multiscale analysis, especially considering this model at more than one scale of observation, which indicates a gap in knowledge. In this respect, the purpose of this work is to extend a proposal found in the literature for the computational homogenization of the phase-field [1] to problems involving pressurized fractures [2]. Micro and mesoscale will be considered. The microscale is designed to represent the composite material as a heterogeneous medium formed by components with different mechanical properties. The mesoscale is treated as an equivalent medium with homogenized properties. Both scales are modeled by a PFM that considers the pressure load on the fracture surface. Based on this proposal, it is be possible to verify the impact of the transition of the field variables and dual internal variables of the PFM from one scale to another and follow the evolution of the fracture process on two scales. All computational implementation and numerical simulations will be developed in the open-source software INSANE.

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TOPOLOGY OPTIMIZATION FOR FIBER ORIENTATION IN FRACTURED CONCRETE

Andre Luis Ferreira da Silva[*1], Luís A. G. Bitencourt Jr.[1] and Emilio Carlos Nelli Silva[1]*

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ABSTRACT

Concrete is widely used in civil engineering due to its compression strength. However, it is prone to cracking under tension, necessitating reinforcements to mitigate this vulnerability. The addition of fibers in the concrete has been used to improve the concrete resistance under tension solicitation after cracking occurrence. However, the orientation of these fibers plays a crucial role in the structure's mechanical behavior, making it possible to reduce the amount of fibers used to reinforce the concrete. The optimized fiber orientations are addressed in this work using the Topology Optimization.

The concrete behavior is simulated using a Continuum Damage Mechanics Theory (CDMT)-based model with a rate-independent formulation, distinguishing between tensile and compressive responses.

The methodology integrates an implicit-explicit integration scheme to improve computational efficiency. By focusing on the fracture mechanics model, we seek to minimize structure compliance, indirectly extending the lifespan of the reinforced concrete. We present the methodology, results, and conclusions, highlighting contributions to the field of concrete reinforced with fibers.

Analytical models for nonlinear dynamics and evolved dynamics in natural, social and engineering sciences
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COUPLED TWIN CONICAL FUNNELS OR CONICAL HOSES: AN INTERNAL PROCESS OF DYNAMIC FLOW DISTRIBUTION

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ABSTRACT

The analytical derivation of internal dynamic hoses of conical type for conical flow takes place from the Laws of Continuity, Momentum and Energy. This analytical derivation is the objective of this article. From the physical laws of fluid mechanics, some evidence is obtained for two non-classical analytical boundary conditions necessary for this phenomenon. After these two new boundary conditions and since supersonic and hypersonic solid cones are related to theoretical and industrial interest, new analytical regions are established and characterized in the graph of cone angle, shock angle and Mach number of free flow.

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EVOLVING DYNAMICS FOR THE ANALYSIS OF COMPLEX CRATERS

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ABSTRACT

In this work, dynamics evolution models are developed for the analysis and interpretation of processes, properties and temporal distribution of the matter involved in the formation of complex craters. The laws of fluid dynamics are applied as a tool for the development of the analytical model that allows subsequent analysis. The high energy process that is analyzed and described is explained through the evolution of dynamic balances associated with new energy balances in stages and related to a sequence of configurations that constitute patterns and geometries that evolve together with the dynamics of the formation of a complex crater. Then, the described dynamics involves considering stages, times, shapes, speeds, energies, impacts, frictions, rebounds and mass losses to develop the new model. As a consequence, at least three emergent physical phenomena are identified: a traveling piston (matter in motion in the process of melting), concentric rings and a raised central formation. Physical laws and phenomena are combined to obtain an energy distribution. Finally, a dynamic and thermodynamic balance is carried out in perspective and applied to known craters that are representative of the formation of complex craters and a good correlation is verified with the quantitative results predicted by the developed model

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Advances in computational biomechanics and mechanobiology
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREGNANCY BEFORE THE ONSET OF LABOR: A HOLISTIC BIOMECHANICAL PERSPECTIVE

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ABSTRACT

The success of pregnancy and vaginal delivery is highly dependent on the complex interaction between the uterine body, cervix, and fetal membrane [1]. Usually, this interaction is synchronized, following a specific sequence in normal vaginal deliveries: (1) cervical ripening, (2) decidual activation/rupture of fetal membrane, and (3) uterine contractions [2]. Serious complications during vaginal delivery may occur when this sequence is not followed, such as difficult labor progression [2]. Understanding the phenomena occurring during the late stages of pregnancy is essential to offer clinical guidance and solve these problems.

This work analyzes the complex interaction between the cervix, fetal membrane, and uterine contractions before the onset of labor using a complete third-trimester gravid model of the uterus, cervix, fetal membrane, and abdomen. Through a series of numerical simulations, we investigate the impact of (i) initial cervical shape, (ii) cervical stiffness, (iii) cervical contractions, and (iv) intrauterine pressure on the resultant cervical shape and fetal membrane stress during uterine contractions.

The findings reveal several key observations: (i) maximum principal stress values in the cervix decrease in more dilated, shorter, and softer cervices; (ii) reduced cervical stiffness produces increased cervical dilation, larger cervical opening, and decreased cervical length; (iii) the initial cervical shape impacts final cervical dimensions; (iv) cervical contractions increase the maximum principal stress values and change the stress distributions; (v) cervical contractions potentiate cervical shortening and dilation; (vi) larger intrauterine pressure (IUP) causes considerably larger stress values and cervical opening, larger dilation, and smaller cervical length; (vii) the biaxial strength of the fetal membrane is only surpassed in the cases of the (1) shortest and most dilated initial cervical geometry and (2) larger IUP.

This is the first numerical study embracing a complete full gravid uterine and cervical model, uterine and cervical contractions, and a diversity of features associated with pregnancy. We hope to gain more insight into what conditions may influence a successful vaginal delivery and clarify the complex interaction between the cervix, fetal membrane, and body of the uterus, which is not entirely understood.

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Imaging-based methods in computational medicine
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NEW FORMULATIONS FOR DIGITAL TWINNING IN BIOFLUIDS

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ABSTRACT

In biofluids, Digital Twinning relies on leveraging medical images and pressure and flow data to perform customized, subject-specific predictions. Flows in blood vessels and lymphatic systems include complex structured fluids, composed of a liquid phase (plasma) and a disperse phase, which includes cells and other particles such as thrombus. In this work, we present two novel numerical formulations for digital twinning in biofluids, implemented in the open-source framework CRIMSON [1].

In the first application, we are concerned with the study of conditions in which the complex interactions between plasma and suspended particles is required. We recently developed a volume-filtered Eulerian-Lagrangian strategy that uses a finite element method (FEM) to solve for the fluid phase coupled with a discrete element method (DEM) for the particle phase [2].

In a second application, we are concerned with the diagnosis of vascular disease in the catheterization laboratory. Here, images and other hemodynamic data are acquired in real time, and the cardiologist must decide in just a few minutes whether the blockage in the vessels is severe enough to warrant intervention. This application relies on computational tools to accurately estimate pressure gradients and other parameters within minutes. This goal can only be achieved via suitable reduced order models. Our group has recently developed a machine learning approach for calculating pressure gradient indices in image-based vascular models [3].

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Modeling and learning of structured dynamical systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STRUCTURE-PRESERVING INFERENCE OF MECHANICAL SYSTEMS

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ABSTRACT

The construction of mechanical models based on experimental or simulation data is becoming increasingly important in engineering practice. On the one hand, the mechanical models identified from experimental measurements can be used for analysis and simulation. On the other hand, the models used in modern simulation software often need to be further reduced and reconstructed from the simulation results because the original system operators are difficult or impossible to access. Moreover, the identified mechanical system should be able to represent the system behavior for different load cases and time schemes, which means that the original system properties and structural characteristics should be preserved. The recent non-intrusive methods, such as operator inference, often either do not satisfy the latter condition or do not provide a complete system representation due to the specific second-order ODE structure of the governing system of equations. In our work, we propose a methodology for identifying and reducing mechanical systems from data by solving an optimization problem using the capabilities of machine learning techniques. We are able to identify all system operators and preserve their original mathematical properties by including a reasonable parameterization of the system operators in the optimization problem. For linear mechanical systems, this ensures stability and interpretability of the resulting surrogate model. In addition, we study systems with nonlinear material behavior and the possibility of applying non-intrusive reduction methods to them. Numerical experiments are performed using simulation data from finite element software.

Computational and analytical advances in nonlocal modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A VERSATILE COMPUTATIONAL FRAMEWORK FOR CONTINUUM-KINEMATICS-INSPIRED PERIDYNAMICS USING HYPER-DUAL NUMBERS

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ABSTRACT

Continuum-kinematics-inspired peridynamics (CPD) has been recently proposed as a novel reformulation of peridynamics that is characterized by one-, two- and three-neighbor interactions.
CPD is geometrically exact and thermodynamically consistent and does not suffer from zero-energy modes, displacement oscillations or material interpenetration. In this presentation, we introduce a computational framework furnished with automatic differentiation for the implementation of CPD. Thereby, otherwise tedious analytical differentiation is automatized by employing hyper-dual numbers (HDN). This differentiation method does not suffer from round-off errors, subtractive cancellation errors or truncation errors and is thereby highly stable with superb accuracy being insensitive to perturbation values. The proposed computational framework is compact and model-independent, thus once the framework is implemented, any other material model can be incorporated via modifying the potential energy solely. Finally, to illustrate the versatility of our proposed framework, various potential energies are considered and the corresponding material response is examined for different scenarios.

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Uncertainty quantification and scientific machine learning for predictive modeling of complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODEL PARAMETER IDENTIFICATION IN SIMULATIONS OF THE WEST AFRICAN MONSOON WITH THE USE OF SURROGATE MODELS

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ABSTRACT

Numerical simulations of the West African monsoon (WAM) system are subject to substantial uncertainties and challenging to assess due to complex interactions within the circulation system, in particular with respect to clouds. In a previous study, we identified major uncertainty contributors in WAM simulations using the ICON (Icosahedral Nonhydrostatic) model, operationally employed by the German weather service (DWD) [1]. We selected six model parameters with significant uncertainty impacts and 15 Quantities of Interest (QoIs) characterizing the WAM system, including averaged temperature, precipitation, cloud cover, jet speeds and latitudes. We developed surrogate models via universal kriging to establish a relationship between the model parameters and the QoIs. In global sensitivity analyses (GSA), we quantified the uncertainty contributions of these parameters to the QoIs.

In this talk, we will present methods to identify optimal model parameters by incorporating reanalysis data as a reference for the QoIs and output fields. Our analysis is divided into two categories: (1) optimizing QoIs using obtained surrogate models, and (2) optimizing output fields based on grid-point data. These tasks are approached as multi-objective optimization problems, where multiple QoIs or output fields are optimized simultaneously. We tackle this through two novel strategies: (a) assigning weights with uncertainties to QoIs or output fields based on expert opinion and (b) independently varying these weights to assess their impact on the optimal model parameters.

This approach not only integrates expert judgment into model optimization but also enables a dynamic assessment of how weight selection influences the optimal parameters. Our findings reveal a high sensitivity of the optimal parameter set to the assigned weights, highlighting the critical role of weights in model optimization.

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Data-driven methods for modeling complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ARTIFICIAL INTELLIGENCE IN DAM ENGINEERING

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ABSTRACT

Artificial intelligence has been evolving at an incresing rate. Early adopters are already benefiting from it, and most companies consider implementing artificial intelligence strategic to increase profits and remain competitive. This paper highlights the challenges and opportunities that artificial intelligence presents to dam engineering.

Lots of data are gathered daily by instruments and inspections. Assessing them timely is important to understand the current condition of a dam. Furthermore, the earlier an anomaly is detected, the more likely it is to keep it under control. Artificial intelligence can quickly process large amounts of data and give dam engineers the information they need to find the best solution.

The optimal operation of a gated spillway must consider deterministic and stochastic values. The former are current, whereas the latter are forecast. Many scenarios should be frequently analysed to define what the best gate operation is at each stage. Artificial intelligence allows to consider all of them and select the one that maximises benefits while safeguarding dam safety.

Ground conditions interpretation is time-consuming and is usually carried out once the site investigation is finished. Artificial intelligence can expedite the process, so the remaining part of the campaign can be adjusted based on a preliminary assessment of gathered data. Moreover, the complexity of the generated ground model can be increased to better represent reality.

Those are just a few examples of why artificial intelligence has arisen so much appetite. Dam design, construction, and operation are complex to the point that can overwhelm humans. The challenges that artificial intelligence adoption presents must be overcome for dam engineering to benefit from the opportunities it offers.

Space-time modeling of coupled problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ISOTHERMAL, LINEAR THERMOMECHANICAL COUPLING OF DIFFUSIONAL PHASE TRANSFORMATIONS AND CONSTITUTIVE LAWS TO PREDICT DAMAGE AT SMALL SCALES

Wolfgang Flachberger[*1], Swaroop Gaddikere-Nagaraja[1], Thomas Antretter[1] and Silvia Leitner[2]*

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ABSTRACT

This work presents a Lagrangian formulation for the coupling of diffusional phase transformations and continuum mechanics using the finite element method (FEM). The emphasis on the Lagrange formalism is due to its convenience in automatically deriving variational forms, especially for coupled problems. Although the derived variational form can be used with any Galerkin-type numerical method we present a specific mixed finite element method that employs less comon basis functions such as the "discontinuous Galerkin" and the "Raviart-Thomas" element. The mixed FE approach has beneficial features such as better stability properties and less degrees of freedom in comparison to the usual Galerkin elements. The approach is used to investigate the impact of mechanical stresses on segregation and other damage mechanisms observed at the small scales. The model is characterized by sharp transitions between phases (sharp interface model) which is in strong contrast to other state-of-the-art methods for describing diffusional phase transformations like the Phase Field Method (PFM). It will however be shown that the presented model can actually be interpreted as a limiting case of Cahn Hilliard diffusion (PFM). A binary system is studied whose behaviour is described by four differential equations which are solved by an implicit, fully coupled scheme. The diffusion model is used to predict both the phase growth as well as damage relevant phenomena such as segregation of components at grain boundaries. Furthermore, the diffusion is coupled with a constitutive model for the mechanical material behaviour. The coupling is done in both ways considering the influence of diffusion on mechanics via phase-dependent material parameters as well as by considering the influence of stresses and strains on the diffusion. This enables a detailed investigation of the many phenomena that are observed in nonequilibrium systems.

Physical models and reduced order models augmentation with data for physics-informed machine learning in real-world applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NON-INTRUSIVE HYPER-REDUCTION FOR DYNAMIC NONLINEAR STRUCTURAL FINITE ELEMENTS APPLICATIONS

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ABSTRACT

Several Hyper-Reduction (HR) approaches, such as e.g., the Energy Conserving Sampling and Weighting (ECSW) [1], have been proposed to reduce the computational cost of nonlinear structural Finite Element (FE) analyses. However, many HR approaches are typically intrusive, posing challenges when it comes to integration into existing commercial software. Recently, several data driven methodologies have been proposed to generate Non-Intrusive Reduced Order Models (NIROMs) of nonlinear dynamic FE problems. NIROMs can be obtained via surrogate modelling by learning the dynamic on the reduced space, or via system identification by approximating nonlinear operators [2]. While being non-intrusive, they typically suffer from limitations such as overfitting, a reduced capacity to extrapolate and violation of key physics properties resulting in unstable behaviour.

This work proposes a data-driven, physics-augmented artificial neural network approach based on the Input Convex Neural Network (ICNN) architecture [3] for nonlinear structural FE formulations. The proposed approach combines stability-preserving properties of HR approaches with the non-intrusive properties of data-driven approaches. The resulting NIROM possesses the necessary stability-preserving properties to be successfully employed in dynamic numerical simulations. The proposed approach is validated on a nonlinear structural FE model of a cantilever beam undergoing nonlinear geometrical and material behaviour whilst subjected to different dynamic loads. A Proper Order Decomposition reduced order basis is generated using a set of displacement field snapshots obtained from different dynamic loading conditions, whereas reduced internal force snapshots are used to train the proposed network. The proposed ICNN-based architecture guarantees the a-priori enforcement of physical constraints and therefore provides stable and consistent predictions, unlike e.g., Fully-Connected NN approaches. The obtained results highlight the efficiency of the proposed approach for dynamic structural FE problems and showcase its potential as well for parametric and multiphysics applications.

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COMPUTATIONAL MODELING OF EXPLOSIVELY DRIVEN FLYER PLATE EXPERIMENTS IN ALEGRA

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ABSTRACT

The Light Initiated High Explosive (LIHE) facility at Sandia National Laboratories conducts experiments that utilize LIHE to evaluate the response of structures to shock loading. One version of the experiment consists of accelerating a thin metal flyer plate into a target material, delivering a prescribed impulsive load to the target.

During the experiment, the flyer plate is accelerated by the detonation of silver acetylide silver nitrate (SASN) explosive applied to the flyer plate surface. SASN is a highly sensitive primary explosive and can be simultaneously initiated over the sprayed flyer plate surface by an intense flash of light.

The impulse delivered to the target material is a direct function of the SASN explosive deposition on the surface of the flyer plate, the flyer plate material/thickness, and the initial air gap between the flyer plate and impact surface of the target material. By tailoring these parameters, the experiment can be designed to deliver the desired impulse to the target material.

As the LIHE flyer plate technique has matured, work has been done in parallel to build high-fidelity computational models to better inform the design of experiments. A 2D axisymmetric finite element model of the flyer plate experiment was developed in ALEGRA, an arbitrary Lagrangian-Eulerian multi-physics code. The model accounts for the detonation of the explosive, expansion of the detonation products, and the motion and mechanical deformation of the flyer plate. The ALEGRA simulations show good agreement with provided experimental data for the flyer plate velocity as it accelerates, impacts the target material, and rebounds. This work summarizes the development of the ALEGRA computational model and the results.

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Simulations of particle-laden fluid flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL ANALYSIS OF SOIL EROSION WITH MATERIAL POINT METHOD AND NON-CONFORMING RIGID LINE MODELING

Anthony Flores[1], Luis Zambrano[1] and Bill Davids[1]*

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ABSTRACT

Soil erosion poses challenges in engineering that require mitigation to ensure the safety of structures, protect natural resources, and plan sustainable projects. The analysis of soil erosion from an engineering perspective is complex as it is composed of the soil-water or soil-air interaction, where each component is dependent on mechanical parameters that have been empirically quantified, lacking theoretical soundness due to the complexity of the phenomena described. One of these parameters is the soil frictional stress, which is a crucial input for measuring both local and global scour, influenced by the velocity gradient of water flow, and it lacks an analytical solution, necessitating numerical methods. While widely used, the conventional finite element method (FEM) has limitations in capturing long deformations and post-failure behavior. Furthermore, it often relies on aggressive and expensive algorithms.

A bidirectional contact algorithm between the rigid element and the particles has been integrated into the Anura 3D software. The Material Point Method (MPM) has been selected due to its ability to simulate large deformations while effectively tracking the behavior of individual particles. A simplified 2D analysis of an open sea where water particles engage with a soil layer has been considered. A rigid line element moving rotationally is proposed to simulate the water wave, with its lower edge serving as the center of rotation. This algorithm enables the creation of rigid 1D-line elements not conforming with the background mesh. Contact detection is then carried out through a distance field assigned to each material point, considering a radius of influence for each material point based on its density. Subsequently, a Lagrangian correction is applied to the rigid body, followed by an Eulerian correction to the material points, ultimately proceeding with the standard MPM cycle.

A model with a soil and a liquid layer has been developed to test the contact algorithm. The model included a rigid body that was a mechanical simulation of waves in the liquid.

Computational modeling of cardiac fibrosis: A multiscale, multiphysics challenge
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTI-FIDELITY, MULTI-PHYSICS MODELS OF FIBROSIS-INDUCED LEFT ATRIAL THROMBOSIS

Manuel Guerrero-Hurtado[1], Yvonne Stöcker[2], Alejandro Gonzalo[3], Clarissa Bargellini[3], Bahetihazi Maidu[3], Eduardo Duran[4], Pablo Martinez-Legazpi[5], Javier Bermejo[6], Andrew M. Kahn[7], Elliot McVeigh[7], Manuel García-Villalba[2], Nazem Akoum[3], Christoph Augustin[8], Patrick Boyle[3], Juan C. del Álamo[3] and Oscar Flores[1]*

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ABSTRACT

Ischemic strokes are a significant cause of mortality and long-term disability in patients with atrial fibrosis. However, the underlying mechanisms are not understood and there are no predictive tools for clinical decision support, even if atrial fibrosis can be assessed non-invasively with imaging modalities like late gadolinium enhancement magnetic resonance imaging (LGE-MRI). Fibrotic remodeling modifies myocardial structure impairing LA electrical propagation, myocardium mechanics, and slowing down atrial blood flow. In addition, fibrotic patches release inflammatory cytokines and tissue injury factors that can activate the coagulation cascade.

To evaluate the role of these effects and their potential interactions, we perform multi-physics simulations, coupling electrophysiology, biomechanics, hemodynamics, and the coagulation cascade. We significantly reduce the computational cost of these simulations with two innovations. First, we introduce a multi-fidelity approach leveraging the low molecular diffusivity of coagulation species, which accelerates the simulation of reaction advection equations by over one order of magnitude. Second, the resulting modular multi-physics solver is implemented to run in graphics processing units (GPUs), achieving an additional speedup of almost two orders of magnitude. Overall, these innovations reduce the cost of the multi-physics simulations to ~ 1h per cardiac cycle, reducing the gap between the time associated to clinical diagnosis tests and the time to run patient-specific simulations.

We use these multi-physics simulations to analyze patient-specific models with different fibrosis burdens based on LGE-MRI scans. Fibrotic regions are modeled by locally modifying the myocardial mechanical properties and releasing pro-coagulatory tissue factor in the neighboring endocardium. To elucidate the interplay between these effects, the following conditions are considered per patient-specific model: no fibrosis, 5X increased passive stiffness and 2X reduced cardiomyocyte contractility (mechanical disruption), tissue factor release in fibrotic patches with normal mechanical properties (pro-coagulatory disruption), and both mechanical and pro-coagulatory disruption. These simulations will shed light onto

the complex nexus between fibrosis and stroke. Furthermore, their reduced computational cost is poised to create paradigm changes in clinical diagnosis support and personalized therapeutic planning.

Analytical models for nonlinear dynamics and evolved dynamics in natural, social and engineering sciences
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DYNAMICS OF THE RELIABILITY OF AN AERIAL SYSTEM OPERATING IN ADVERSE CONDITIONS

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ABSTRACT

Aerial systems must comply with basic capabilities to ensure the continuity of their operation under acceptable conditions and particularly in adverse situations. This is how, within a dynamic framework, reliability and degradation models are essential for prediction and decision making. Its application and execution provides results that, compared with historical measurements, allow the evaluation of the prediction and, if satisfactory, allows for an acceptable state of security based on the predictive tool which, by its nature, provides probable results in a simple way, early and continuous.
The necessity to know the system degradation´s speed on one hand and when to provide the necessary logistical support to restore it on the other hand, is a frequent problem in the aeronautical sector that occurs mainly for safety reasons for both the operator and the its human and material environment.
In this context, we recognize unavoidable and at the same time contributing aspects, which interact with each other and where we distinguish various operating variables, both endogenous and exogenous to the system, which by themselves generate a possible set of desired values for efficient, effective and safe work that allow the aerial system maintenance. From there, we also analyze the different responses in relation to their recovery capacity and they are quantified in this work in probabilistic terms. It should be noted that, even moving in a region where the quality is desired, the demanding uninterrupted operation of the system is associated with failure and degradation which requires periodic restoration of high, medium and low frequency (corrective, restorative and preventive) facilitated by the developed model. However, the sustained activity of the system causes a growing accumulation of tensions that occur in order to renew the daily availability of the system, causing an essential effort that is also increasing to sustain the permanent functioning of the system. The result is that the system degrades to such an extent that it limits the extent of its activity over time.
In this paper we propose models for the timely prediction of restoration moments, which maximize the useful life of the system conceived from its endogenous and exogenous variables. Finally, real cases with different responses are analyzed in an environment associated with countries where resources are not abundant or in systems that for functional reasons are self-sufficient degenerative or, at the same time, operate in adverse environments.

LANDSLIDE RUN-OUT SIMULATIONS WITH DEPTH-AVERAGED MODELS AND INTEGRATION WITH 3D IMPACT ANALYSIS USING THE MATERIAL POINT METHOD

Marco Fois[1], Carlo de Falco[1], Andi Makarim Katili[2], Antonia Larese[3] and Luca Formaggia[1]*

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ABSTRACT

Landslides pose a significant threat to human safety and the well-being of communities, making them one of the most challenging natural phenomena. Their potential for catastrophic consequences, both in terms of human lives and economic impact, is a major concern. Additionally, their inherent unpredictability adds to the complexity of managing the risks associated with landslides. It is crucial to continuously monitor areas susceptible to landslides. In situ detection systems like piezometers and strain gauges play a vital role in accurately monitoring internal pressures and surface movements in the targeted areas. Simultaneously, satellite surveys contribute by offering detailed topographic and elevation data for the study area. However, relying solely on empirical monitoring is insufficient for ensuring effective management of hazardous situations, especially in terms of preventive measures. The substantial economic costs and the impracticality of conducting realistic experiments underscore the growing necessity of developing numerical simulations to better understand and address landslide phenomena. This study provides advanced simulations of mudflows and fast landslides using particle depth-averaged methods, specifically employing the Material Point Method adapted for shallow waters (Depth Averaged Material Point Method). The numerical method has been parallelized for enhanced efficiency and validated through benchmark tests and real-world cases. Furthermore, the investigation extends to coupling the depth-averaged formulation of shallow water with a three-dimensional formulation in order to have a detailed description of the impact phase of the sliding material on barriers and membranes. The multidimensional approach and its validation on real cases provide a robust foundation for a more profound and accurate understanding of the behavior of mudflows and fast landslides.

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Advanced multiscale and adaptive numerical methods for non-linear solids
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADAPTIVE MESH ALGORITHM FOR FRICTIONAL CONTACT PROBLEMS BASED ON A POSTERIORI ERROR ANALYSIS

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ABSTRACT

The finite element method is a widely adopted computational tool for solving problems formulated as partial differential equations in computational mechanics. For instance, engineering teams often perform finite element numerical simulations to analyze the behavior of large hydraulic structures. The nonlinear behavior of concrete dams, particularly within their weakest zones, such as the concrete-rock contact in the foundation or the interfaces between blocks, significantly influence their stability. A mathematical approximation representing the behavior of these zones consists in the unilateral contact conditions with friction, expressed in terms of normal and tangential components of displacement and surface stress at the interface level.

This presentation concentrates on frictional unilateral contact problems within a framework encompassing both Tresca and Coulomb friction conditions. Numerically, we adopt a finite element discretization with weak enforcement of nonlinear contact conditions à la Nitsche. This choice enables an easy implementation of the contact conditions in a weak sense without the introduction of additional unknowns such as Lagrange multipliers. For this problem, we present an a posteriori error analysis based on equilibrated stress reconstruction, providing a guaranteed fully-computable upper bound of the error that distinguishes the different components of the error through some local estimators [1], in the spirit of [2]. The key concept behind these estimators is to provide an equilibrated stress reconstruction with continuous normal trace across the edges of the mesh, locally in equilibrium with the volumetric and surface forces. Inspired by [3], we propose a practical method to achieve this reconstruction by assembling solutions of problems locally defined on patches around mesh vertices using the Arnold-Falk-Winther mixed finite element space.

We use then the local estimators to introduce a fully-automated adaptive algorithm for the refinement of the mesh with a stopping criterion for the linearization algorithm. Numerical compare this adaptive algorithm with a uniform approach, showing that the former provide better convergence rate for the error measured in the H1-norm and energy norm.

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THE HODGE-LAPLACIAN ON DOUBLE COMPLEXES GOVERNS COUPLED PROBLEMS

*Daniel Førland Holmen**[1], Jan Martin Nordbotten[1], Jon Eivind Vatne[2] and Wieste Marjin Boon[3]*

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ABSTRACT

The de Rham complex unifies the treatment of the classical differential operators in vector calculus, in particular the gradient, curl and divergence in three-dimensional space. When the complex is equipped with inner products we obtain the Hodge-Laplacian, generalizing the usual scalar/vector Laplacian. Thus, the study of cochain complexes is strongly linked to certain processes in continuum mechanics governed by partial differential equations.

Recent work has established that various coupled problems can also be cast in the context of (double) cochain complexes. The Hodge-Laplacian on the mixed-dimensional de Rham complex describes coupled problems where the coupling takes place across manifolds of various dimensions [1]. On the other hand, the Čech-de Rham complex is a cochain complex where the coupling is on an equidimensional overlap of domains. It has been shown that Hodge-Laplacians on the Čech-de Rham complex corresponds to models of coupled problems common in applications [2].

A cochain map between the mixed-dimensional de Rham complex and the Čech-de Rham complex can therefore be seen as a link between mixed-dimensional and equidimensional representations of the same physical problem. The construction of the aforementioned cochain map have been made for a class of mixed-dimensional geometries [3]. Additional properties of such a cochain map will lead to an approximation theory between mixed-dimensional and equidimensional models.

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Efficient numerical methods for CFD and FSI simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A DEPTH AVERAGED MATERIAL POINT METHOD FOR FAST FLOW-LIKE LANDSLIDES AND MUDFLOWS

Luca Formaggia[*1], Marco Fois[1], Carlo de Falco[1] and Simona Perotto[1]*

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ABSTRACT

Among the most dangerous natural phenomena for the safety of people, landslides are one of the most problematic: not only because of their potentially catastrophic nature in terms of human and economic loss, but also because of their intrinsic unpredictability.

In this work, we are interested in the development of efficient tools for the simulation of landslide evolution immediately following the phase of initiation of the landslide front. The basic mathematical model used to describe gravity-driven free surface flows is the depth-integrated equations derived from the Navier-Stokes equation for an incompressible fluid. We propose a semiconservative variant of the Depth-Averaged Material Point Method (DAMPM), which is a depth-integrated version of the Material Point Method (MPM). Numerical test are carried out to verify the effectiveness of the procedure both on synthetic and real case scenarios.

Computational and analytical advances in nonlocal modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SYMMETRY FOR OPEN SETS WITH ORDERED NONLOCAL CURVATURE

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ABSTRACT

This talk will focus on a geometric problem involving nonlocal mean curvature defined via an integrable kernel. In the classical setting, it is well known that a smooth boundaryless surface with constant mean curvature must be a sphere. Li and Nirenberg studied the problem where the mean curvature is instead assumed to be monotone (ordered) in a given direction. Under certain geometric and regularity assumptions, they showed there must be a hyperplane, orthogonal to that direction, across which the surface is symmetric. Thus, if the mean curvature is ordered in all directions, the surface is a sphere. I will present an analogous result where the curvature is measured with a nonlocal operator and the surface is the boundary of an open set.

Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL MODELING OF DEEP EARTHQUAKES CONSIDERING PHASE TRANSFORMATION AND THERMAL EFFECTS

Craig Foster[*1], Sheng-Wei Chi[1], S Sindhusuta[1], Ashay Panse[1], Javad Mofidi Rouchi[1], Yanbin Wang[1] and Timothy Officer[1]*

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ABSTRACT

The causes of deep earthquakes, those below approximately 60 km, remain poorly understood. High pressures prohibit the frictional sliding that dominates shallower earthquakes. Roughly, these earthquakes are split between intermediate-depth earthquakes, those between 60 and 350 km depth, and deep-focus earthquakes, those below 350 km. These two types of earthquakes seem to be clustered distinctly by depth and may have different mechanisms.

One of the leading hypotheses, especially for deep-focus earthquakes, is that of transformational faulting. Under high temperatures and pressures, minerals in the subducting slab change phase to denser and weaker structure. The densification can remove some of the pressure on the material and, combined with weakening, allow for sliding. High strains along the band can start to create transformation in narrow bands. Thermal effects can also locally enhance phase transformation, creating a runaway reaction that could lead to a macroscale event.

We create an enhanced finite element model to model these processes and see if macroscale fault generation is possible by this mechanism. Phase transformation is modeled as a rate process that is a function of temperature and mean stress, following [1]. Under the correct softening conditions, the phase transformation can localize into narrow bands. These bands are modeled using an enhanced strain finite element.

We first model small laboratory experiments [2] to see if local inclusions can perturb the stress field enough to incite this process. We then upscale the model to examine fault-scale scenarios, to see if large-scale earthquakes can be generated at depth. These simulations will eventually be compared to catalogs of deep earthquakes to see if they match the characteristics of observed events.

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16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics

July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE HUNTER, THE RANCHER, THE RENAISSANCE MAN: A TRIBUTE TO MY BELOVED FRIEND TINSLEY ODEN

*John Foster**[1]

[1]*The University of Texas at Austin*

ABSTRACT

Over the last eight years of his life, I spent considerably more time at "Oden Ranch" with Tinsley than on campus. We would traverse the ranch's expansive terrain, covering more than 10 miles of dirt, rock, and hilly roads in his well-worn Ford F250, which spanned nearly 800 acres. As we attended to ranch duties, I was captivated by his tales of adventure. His stories ranged from hunts in the Arctic Circle to expeditions in Africa and South America, not forgetting the countless autumn deer hunts on the ranch. He had an incredible memory for the names and personalities of guides and guests who joined him on these adventures.

Though Tinsley was globally recognized for his professional achievements, I will always cherish his genuine affection and kindness towards everyone he met, especially those who shared his passion for the outdoors, myself included. In this talk, I aim to recount some of the stories he shared with me, as well as those we forged together. These narratives will be accompanied by photographs and, quite likely, some tears, as I pay homage to my dear friend.

16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Advances in discretization techniques, element technology, mesh adaptivity, and solution strategies for inelasticity, localization, and failure

July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADVANCES IN A 10-NODE COMPOSITE TETRAHEDRAL FRAMEWORK FOR SHOCK AND MESH ADAPTIVITY

James Foulk[1], Jesse Thomas[1], Scott Miller[1], David Noble[1], William Scherzinger[1], Michael Veilleux[1] and Alejandro Mota[1]*

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ABSTRACT

We have extended the recently reformulated 10-node composite tetrahedral finite element for solid mechanics. We generalized the gradient operator and mass matrix to curved domains through analytical expressions weighted by subtetrahedra Jacobians. Optimal integration weights were constructed to increase the accuracy of Gaussian quadrature. We preserved the variational structure of the formulation through a new five-field functional with additional, independent fields for the Jacobian and the pressure. A deleterious soft mode, common to both the quadratic and composite tetrahedral element with constant pressure formulations was effectively stabilized through a novel convex energy penalty function.

In recent work, we probed the viability of the formulation for shock. We investigated a new, nonlinear, symmetric stabilization scheme for structured and unstructured meshes. The new scheme enables the large volumetric strains inherent in shock environments and does not affect prior work focused on large, unconfined, plastic deformations.

Here we extend the requisite stabilization schemes to mesh adaptivity. We focus on new methodologies for mapping the stabilization energy to a stressed reference configuration and examine the impact on the solution. We explore problems of increasing complexity for metals that span convergence for Taylor bar impact to resolving Richtmyer-Meshkov instabilities.

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Data-driven device and circuits models
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTIMODAL, DATA-DRIVEN MODELING OF INTERDIGITATED COMB SENSORS FOR CHARACTERIZATION OF ELECTRONICS RELIABILITY

James Fowler[*1], Matthew Kottwitz[1], Rosario Gerhardt[2], Roshaun Titus[2], Anthony Trofe[13], Samuel Grosso[41], Ayorinde Olatunde[5], Kristopher Davis[6], Jarod Kaltenbaugh[6] and Fernando Garzon[41]*

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[3]*Joint School of Nanoscience and Nanoengineering*
[4]*University of New Mexico*
[5]*Case Western Reserve University*
[6]*University of Central Florida*

ABSTRACT

Surface insulation resistance (SIR) serves as an IPC J-STD-001H prescribed method of obtaining objective evidence that manufacturing processes for high performance/harsh environment electronic products result in acceptable levels of residues such that performance under anticipated operating conditions is not adversely affected. Despite this methodology providing potential insight into the underlying physical phenomena occurring within the system, evaluation of the cleanliness and reliability of a manufacturing process via SIR testing currently relies upon a binary pass/fail paradigm based upon whether the measured current was above a scientifically arbitrary threshold value at any time during the test window. Sandia National Laboratories, in collaboration with university and industry partners, has engaged in a systematic investigation of SIR towards an understanding of how the underlying mechanisms manifest in the observed time-series data. The explored parameter space included (a) design geometry of the test patterns, (b) materials selection in the test board construction, (c) chemistry and concentration of contaminants on the test board and (d) environmental conditions of the test chamber. Additional characterization techniques —electrochemical impedance spectroscopy, capacitance-voltage, more—were conducted before, after and/or in parallel to complement the SIR measurements. Results were interpreted through multivariate statistical analysis and within the context of analytical and equivalent circuit models. Future work seeks to enhance applicability to industry processes through the investigation of increasingly relevant test pattern designs, materials selection, and investigated contaminants.

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A DEEP MATERIAL NETWORK USING MICROPOLAR MECHANICS

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[1]University of Colorado Boulder
[2]Sandia National Laboratories
[3]Los Alamos National Laboratory

ABSTRACT

The deep material network (DMN) is a recent paradigm that combines homogenization techniques with neural networks to rapidly predict the response of composite materials with high accuracy. These reduced order models have analytical formulas at their core, making them capable of extrapolating to other constitutive equations after training only once on linear elastic data. Thus far, the approaches to DMN use classical continuum mechanics to construct the network. Here we study the DMN idea extended to micropolar mechanics, which generalizes the classical continuum to include not only the three displacement degrees of freedom at every point, but three additional microrotation ones too. In the micropolar setting, intrinsic length scale effects representing the microstructure of the material arise naturally. These length scales are not captured in the classical models, so it is of interest to have a DMN sensitive to these effects. The homogenization building block of the micropolar DMN is derived via asymptotic homogenization applied to a simple micropolar laminate. This formula is a function of the normal vector of the laminate plane and the volume fraction; both of which will serve as network parameters to be learned in the training process. The training data is generated using linear elastic micropolar fast Fourier transform (FFT) direct numerical simulations (DNS). Then, using a nonlinear micropolar constitutive model, the micropolar DMN is shown to extrapolate accurately without retraining. The reference DNS used as our metric for accuracy is a nonlinear extension of the micropolar FFT DNS.

Recent advances in computational fracture mechanics and failure analysis
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

UTILIZING MACHINE LEARNING FOR CRACK GROWTH RATES PREDICTIONS IN AN AERONAUTICAL ALUMINUM ALLOY

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ABSTRACT

Recent progress in computational capabilities introduces a new era where data-driven methodologies play a pivotal role in accurately simulating intricate engineering phenomena. These methodologies, harnessing the power of machine learning, offer mathematical approximations that act as surrogate models. Their strength lies in their ability to replace convoluted explicit mathematical relationships with models demanding significantly reduced computational resources.

This study addresses the formidable challenge of predicting the crack growth behavior of aluminum 7075-T6, a commonly used material in the aviation industry. The inherent complexity of crack growth in this alloy stems from several influencing factors, rendering explicit mathematical equations inadequate for comprehensive descriptions. Notably, the presence of "waviness" behavior within the linear Paris law region and the pronounced impact of variables such as the R-ratio and specimen thickness contribute to the intricate nature of crack growth predictions.

To overcome these challenges, we explore four distinct machine learning regression algorithms: Random Forest (RF), Gaussian Process Regression (GPR), K-Nearest Neighbors (KNN), and Kernel Regression (KR). These algorithms are studied for their efficiency in capturing the patterns inherent in the crack growth behavior of aluminum 7075-T6. The performance evaluation involves a meticulous assessment of their predictive capabilities under various conditions.

The key objective is to identify the most promising algorithm among the four, capable of providing accurate and reliable predictions for the crack growth in aluminum 7075-T6 across diverse fatigue stress spectra. By systematically comparing and contrasting the performance of these machine learning algorithms, we aim to shed light on the most suitable approach for tackling the complex task of crack growth prediction in this critical aviation material. This research not only contributes to the understanding of material behavior but also holds the potential to enhance the reliability and safety of aeronautical structures through more informed predictions of crack growth rates.

Uncertainty quantification in structural dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

POLYMORPHIC UNCERTAINTY QUANTIFICATION IN STRUCTURAL DYNAMICS

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ABSTRACT

The reduction of material consumption required to build engineering structures leads to an increasing design of lightweight structures. Optimization approaches can be used to minimize the amount of construction material. However, it is important to investigate the structural performance of lightweight structures under dynamic loads with respect to the structural reliability and serviceability. This requires to quantify the uncertainty of the structural loads and the structural parameters. In this contribution, a concept is presented to consider aleatory and epistemic uncertainty [1] in order to compute the responses of structures under dynamic loading. Stochastic and non-stochastic uncertainty models, such as random variables, intervals and fuzzy numbers, are combined, which leads to a polymorphic uncertainty quantification of the structural performance by means of probability boxes or fuzzy random variables. To compute the uncertain structural responses, a nested loop of Monte Carlo simulations and interval analyses is required, which may be time consuming in case of computational expensive simulation models, e.g., finite element simulations and low probabilities to be computed. To reduce the computation time, surrogate modeling approaches for the finite element simulation model or methods where the failure probability is estimated by the standard deviation are helpful, see e.g. [2]. It is important to capture the time-variant structural behavior within the surrogate modeling approach in case of dynamic loads. The resulting polymorphic uncertain structural responses, such as time series of stresses and accelerations or its maximal quantities, computed by the surrogate model are finally evaluated by means of statistical measures, such as mean values, standard deviations or quantile values. Or they are used to calculate imprecise probabilities of the structural failure with respect to safety and serviceability. Academic examples are presented and the developed approach is applied to a footbridge structure considering the dynamic loads of moving pedestrians, see [3].

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Verification techniques in computational physics and applied mathematics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CODE-VERIFICATION TECHNIQUES FOR INTEGRAL EQUATIONS

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ABSTRACT

Code verification is an important step towards establishing the credibility of the results of computational physics codes. Through code verification, the correctness of the implementation of the numerical methods is assessed. The discretization of differential, integral, or integro-differential equations incurs some truncation error, and thus the approximate solutions produced from the discretized equations will incur an associated discretization error. If the discretization error tends to zero as the discretization is refined, the consistency of the code is verified. This may be taken a step further by examining not only consistency, but the rate at which the error decreases as the discretization is refined, thereby verifying the order of accuracy of the discretization scheme. The correctness of the numerical-method implementation may then be verified by comparing the expected and observed orders of accuracy obtained from numerous test cases with known solutions.

Exact solutions are limited and may not sufficiently exercise the capabilities of the code. Manufactured solutions are a popular alternative, permitting the construction of problems of arbitrary complexity with known solutions. Through the method of manufactured solutions (MMS), a solution is manufactured and substituted directly into the governing equations to yield a residual term, which is added as a source term to coerce the solution to the manufactured solution.

Integral equations yield an additional challenge. While analytical differentiation is straightforward, analytical integration is not always possible. Therefore, the residual source term arising from the manufactured solution may not be representable in closed form, and its implementation may be accompanied by numerical techniques that carry their own uncertainties. Furthermore, in many applications, singular integrals appear, which can further complicate the numerical evaluation of the source term. Therefore, many of the benefits associated with MMS are lost when applied to integral equations in a straightforward manner.

Integral equations incur numerical error from three sources: domain discretization, solution discretization, and numerical integration. Domain-discretization error arises from the approximation of curved surfaces with planar elements. Solution-discretization error arises from the approximation of the solution in terms of a finite number of basis functions, or alternatively the approximation of the underlying equation operators in terms of a finite amount of solution queries. Numerical-integration error arises from the approximate evaluation of integrals, usually with quadrature.

We present our approaches to code verification of integral equations, which isolate and measure these different sources of numerical error. We demonstrate their effectiveness for cases with and without coding errors.

Immersed-boundary variational methods: Theory, data structures, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NEW CONCEPT FOR EMBEDDING SUB-STRUCTURES VIA LEVEL-SETS

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ABSTRACT

A new concept for including sub-structures such as fibres and membranes into bulk materials is proposed and generalized from [1, 2]. The bulk domain is equipped with level-set functions whose isosurfaces and/or isolines represent the geometries of the embedded sub-structures. Each level-set function represents an infinite set of continuously embedded, homogenized sub-structures, implied by each of the infinite level sets. This enables a new concept for advanced, anisotropic materials such as biological tissues, layered rocks, composites, and textiles. Mechanical models are proposed which consider the physics on the individual level sets including the generalization into the whole bulk domain [1, 2]. The bulk models for the sub-structures are coupled to classical homogenous and isotropic mechanical models resulting in a new class of models. For the numerical analysis, the bulk domain is meshed using classical, higher-order elements. It is noteworthy that these elements do by no means align to the embedded level sets which is otherwise characteristic for a fictious domain method. However, the present approach does not come with the usual challenges of FDMs. That is, boundary conditions and numerical integration are done as in the classical FEM and there is no need for stabilization. The numerical approach may be traced back to [3] in the context of transport applications and was called Bulk Trace FEM in [1]. Numerical results confirm the success of the proposed sub-structure models in various contexts, even enabling optimal, higher-order accurate results when smooth solutions are expected.

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Modeling and simulation of coupled processes in geological media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AUGMENTED LAGRANGIAN METHOD FOR FRICTIONAL CONTACT ON FAULTS AND FRACTURES IN POROELASTIC MEDIA

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ABSTRACT

Numerical simulations serve as invaluable tools to study complex subsurface systems and support decision-making. Achieving accurate and reliable simulations for various applications—ranging from carbon storage to geothermal energy production—is contingent upon modeling the concurrent interplay of different physical processes. This includes evaluating hazards such as excessive subsidence or induced seismicity. The core challenge stems from the complex interplay and strong non-linearity intrinsic to these processes. Hydrodynamical properties, for example, are tightly coupled with mechanical configurations, making it challenging to solve with decoupled approaches. As a result, there is a need for robust numerical models capable of reliably predicting the complexities inherent in subsurface systems.

In this work, we propose low-order continuous finite elements to simulate solid matrix deformations, and a cell-centered finite volume discretization to solve both the solid matrix and fracture fluid mass balance equations. Frictional contact is addressed using the augmented Lagrange multiplier method following a conformal approach. A single grid is utilized for both mechanical and flow processes, employing piecewise-constant basis functions for fluid pressure and Lagrange multipliers. The implementation of the augmented Lagrangian method follows a Uzawa procedure—a dual-loop algorithm solving the weak form in terms of displacements and pore pressure, holding the Lagrange multipliers constant in the inner loop and updating them in the outer loop. This method can be viewed as a sort of Lagrange multiplier formulation regularized by penalty functions and it offers distinct advantages. Unlike traditional penalty methods, it avoids increasing ill-conditioning of the linear systems, ensuring numerical stability and converging precisely to the exact solution for a finite value of the penalty coefficient. Additionally, this approach generates a smooth energy functional and transforms the problem into a fully unconstrained one, eliminating the need for an active set strategy typically required when employing the Lagrange Multiplier method.
To validate our approach, synthetic numerical tests demonstrate robustness and accuracy. Furthermore, we apply this methodology to address a real-world problem, demonstrating its practical applicability.

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Computational particle-based solvers for multiphysics & multiscale simulations
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A DEM-SUITED PARALLELIZATION SCHEME

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ABSTRACT

Several approaches have been suggested to enhance high-performance computing of granular flows via the Discrete Element Method (DEM). However, the number of published works on this subject (e.g., [1]) is relatively limited, especially when contrasted with the widespread application of DEM in both research and industry sectors. This scarcity in literature can be attributed to the intrinsic complexity of granular media at the grain scale, which are dynamic and disorganized systems, posing significant challenges to effective parallelization. In our work, we introduce a method that leverages a fundamental constraint of DEM simulations, transforming it into a potential for efficient and adaptable parallel processing on distributed memory systems. Specifically, the "numerical sound speed," determined by the standard particle diameter and the time step, imposes a maximum limit on the speed at which disturbances can travel through the discrete material. We demonstrate how this numerical phenomenon, often considered minor in most applications, can be repurposed as a novel criterion for dividing the spatial domain. This approach fosters a parallelization strategy well-suited for DEM. Our methodology is detailed through its practical integration into the DEM'ocritus software [2,3]. We evaluate its effectiveness via benchmark tests on assemblies of up to 15 million particles. These tests focus on scenarios pertinent to geomechanics and the process industry.

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Contact and interface mechanics: Modeling and computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INTERPOLATION-BASED IMMERSED BOUNDARY FINITE ELEMENT AND ISOGEOMETRIC METHODS FOR MULTI-MATERIAL AND MULTI-PHYSICS PROBLEMS

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ABSTRACT

Immersed boundary methods are high-order accurate tools used to model geometrically complex problems in computational mechanics. While traditional finite element methods require the construction of high-quality boundary fitted meshes, immersed boundary methods instead embed the computational domain in a structured background grid. Interpolation-based immersed boundary methods augment existing finite element software to non-invasively implement immersed-boundary capabilities through extraction. Extraction, which has previously been applied to implement isogeometric analysis (IGA) in finite element codes, interpolates the structured background basis as a linear combination of Lagrange polynomials which can be easily integrated by existing methods. This work extends the previously introduced interpolation-based immersed IGA method [1] to multi-material and multi-physics PDEs, utilizing enrichment schemes analogous to those used in traditional immersed boundary methods like XFEM and XIGA. Beginning from level-set descriptions of domain geometries, Heaviside enrichment is implemented to accommodate discontinuities in the solution field across material interfaces. This allows for image based analysis, which is illustrated in this work by analysis of Micro-CT images of a composite sample. Adaptive refinement, used to both improve interface geometry representations and to resolve large solution gradients near interfaces, is applied with truncated hierarchically-refined B-splines (THB) [2]. Multi-physics problems typically have unique discretization requirements for each field, and fields must be coupled. Extraction allows users to interpolate a variety of discretizations with a single unifying Lagrange basis. Interpolation also provides a straightforward coupling method, both at interfaces and within domains. This work provides numerical examples illustrating optimal convergence rates for this method in both 2D and 3D for PDEs representing heat conduction, linear elasticity, and thermoelasticitiy. We present the utility of this method with an image-based analysis of a composite sample, where in addition to circumventing typical meshing difficulties, our method offers a dramatic reduction in degrees of freedom when compared to classical boundary fitted finite element methods.

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Recent advances in numerical methods for interface problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MONOLITHIC AND PARTITIONED FEM FOR FSI: ALE DIVERGENCE-FREE HDG FLUID SOLVER + TDNNS STRUCTURAL SOLVER

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ABSTRACT

We present novel (high-order) finite element schemes for the fluid-structure interaction (FSI) problem based on an arbitrary Lagrangian-Eulerian divergence-free hybridizable discontinuous Gakerkin (ALE divergence-free HDG) incompressible flow solver, a Tangential-DisplacementNormal-Normal-Stress (TDNNS) nonlinear elasticity solver, and a generalized Robin interface condition treatment. Temporal discretization is performed using the high-order backward difference formulas (BDFs). Both monolithic and strongly coupled partitioned fully discrete schemes are obtained. Numerical convergence studies are performed for the flow and elasticity solvers, and the coupled FSI solver, which verify the high-order space-time convergence of the proposed schemes. Numerical results on classical two dimensional benchmark problems also showed good performance of our proposed methods.

Numerical methods, mathematical modeling and analysis in material science
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHASE-FIELD MODELING OF CRYSTALLITES GROWTH AND POLYCRYSTALLINITY EFFECT ON SOLID-STATE SINTERING

Wenjie Fu[*1], Yongxin Gao[1], Arkadz Kirshtein[2] and Qingcheng Yang[1]*

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ABSTRACT

Crystallite growth and polycrystallinity are crucial determinants of the properties and performance of sintered materials. Understanding their intricate interplay is essential for optimizing manufacturing processes and tailoring material properties to specific applications. In this study, we present a comprehensive phase-field modeling approach to investigate the dynamics of crystallite growth and the influence of polycrystallinity on solid-state sintering.

The phase-field method has emerged as a powerful computational tool for simulating microstructural evolution in materials science. By employing a diffuse interface approach, it enables realistic representation of complex interfaces and morphological changes during sintering. Initially, we validate the recently proposed interracially consistent phase-field model of solid-state sintering by comparing it with experiments involving single-crystal powder materials. Subsequently, we utilize this model to simulate the microstructure evolution of polycrystalline powder particles. We elucidate the mechanisms governing crystallite growth and analyze the effects of grain boundary structure and orientation on sintering kinetics. Our simulations reveal the role of grain boundaries as diffusion pathways and their impact on mass transport during densification.

Overall, our phase-field modeling approach provides valuable insights into the fundamental mechanisms governing crystallite growth and polycrystallinity effects on solid-state sintering. By integrating computational simulations with experimental observations, we aim to facilitate the design and optimization of advanced materials with tailored microstructures and enhanced performance across a wide range of applications.

Inverse and optimization problems for advanced materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INVERSE DESIGN OF PHONONIC CRYSTALS BASED ON PSO-REINFORCEMENT LEARNING COUPLED WITH THE LOCALIZED COLLOCATION METHOD

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ABSTRACT

The development of phononic crystals offers a potential solution for precise control of acoustic/elastic waves. Designing phononic crystals with desired characteristics has become a research focus in recent years. However, the precision of altering acoustic and mechanical waves remains a significant challenge for existing inverse design methods. The rapidly advancing field of machine learning is revolutionizing the design of these materials. As an important branch of machine learning, reinforcement learning is being employed to solve mechanical problems more intelligently through the interaction of an agent with its environment. In this paper, we demonstrate the successful application of machine learning in designing 2D phononic crystals with the desired band structure. We first employed the meshless generalized finite difference method to solve the dispersion equation for a periodic structure. To achieve a desired frequency range with a wider first-order bandgap width, we utilized a modified reinforcement learning algorithm incorporating particle swarm optimization to effectively estimate the shape parameters. This parallel technology offers computational cost savings, is independent of the initial state and target, and is effective and stable. This enhanced reinforcement learning-based interactive design approach can be easily applied to other reverse engineering problems.

Advances in material model calibration for computational solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXTREME SPARSIFICATION OF PHYSICS-AUGMENTED NEURAL NETWORKS FOR INTERPRETABLE MODEL DISCOVERY IN SOLID MECHANICS

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ABSTRACT

Data-driven constitutive modeling with neural networks has received increased interest in recent years due to its ability to easily incorporate physical and mechanistic constraints and to overcome the challenging and time-consuming task of formulating phenomenological constitutive laws that can accurately capture the observed material response. However, even though neural network-based constitutive laws have been shown to generalize proficiently, the generated representations are not easily interpretable due to their high number of trainable parameters. Sparse regression approaches exist that allow for obtaining interpretable expressions, but the user is tasked with creating a library of model forms which by construction limits their expressiveness to the functional forms provided in the libraries. In this work, we propose to train regularized physics-augmented neural network-based constitutive models utilizing a smoothed version of L0-regularization. This aims to maintain the trustworthiness inherited by the physical constraints, but also enables interpretability which has not been possible thus far on any type of machine learning-based constitutive model where model forms were not assumed a-priory but were actually discovered. During the training process, the network simultaneously fits the training data and penalizes the number of active parameters, while also ensuring constitutive constraints such as thermodynamic consistency. We show that the method can reliably obtain interpretable and trustworthy constitutive models for compressible and incompressible hyperelasticity, yield functions, and hardening models for elastoplasticity, for synthetic and experimental data.

New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZED-MECHANICAL UNFEELABILITY REVERSAL

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ABSTRACT

Mechanical unfeelability cloak is a metadevice that can realize mechanical unfeelability which is an analogy of optical invisibility to elasto-mechanics. A mechanical unfeelability cloak, usually surrounding an obstacle that is stiffer than a host material, reproduces a displacement field as if no obstacle is present inside the host structure despite the obstacle is actually present. It is very difficult to apply transformation theory, one of the most common approaches when designing cloaking devices that manipulate different physics, to elastic mechanics because the governing equation is not form-invariant, then, the approach for designing a mechanical unfeelability cloak is very limited. Mechanical unfeelability cloaks are usually composed of mechanical metamaterials which realize anisotropic mechanical properties by tuning the artificial microstructures. Some different schemes have been also proposed based on isotropic bulk materials for mechanical unfeelability cloaking without using mechanical metamaterials. Topology optimization is one of the promising approach to design a mechanical unfeelability cloak, some attempts have been proposed using density based topology optimization and level set-based topology optimization. Recent development of the topology optimization enables not only designing elastic structures for cloaking but also adding an mechanical function to optimum structures such as an mechanical cloak-concentrator. In this work, we propose new multifunctional mechanical structures performing for both cloaking and reversing stress inside. The aim is to minimize the stress in the same direction as the external load as the first objective function, and to make the sign of the objective function negative in order to reverse the stress. To suppress the displacement caused by the reversal system, the difference between cloaked displacement and that of a host homogeneous structure is minimized as the second objective function. Radial Basis Function (RBF) parametrized-level set method is employed as a structural modeling to reduce the number of design variables without sacrificing the accuracy of finite element analyses. A covariance matrix adaptation evolution strategy (CMA-ES) is employed to explore the optimal set of design variables because of its robustness to difficult properties such as multimodality, interdependence between design variables, etc. CMA-ES is a multi-point search that adapts its distribution parameters for sampling, i.e. the shape, size and center of the distribution of candidate solutions generated based on normally distributed-random numbers. The use of CMA-ES makes designers free from guessing the appropriate initial solution and adjusting strategy parameters.

Mathematical modeling and simulation for social, environmental, and disaster prevention issues
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MICRO- AND MACROSCOPIC HYBRID TRAFFIC SIMULATION MODEL FOR HIGHWAY MERGING SECTION

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ABSTRACT

A hybrid traffic simulation model is defined as a combination of multiple traffic models with different resolutions, which are dynamically switched to each other. The proposed model couples a microscopic and a macroscopic model. Macroscopic models aggregate the behavior of many vehicles into macroscopic variables, e.g., density, traffic volume, and mean speed, and update these variables at long intervals. For this purpose, a model that regards the fluid as a continuum is used [1]. Meanwhile, microscopic models individually determine each car's behavior through a series of rules [2]. Here, a traffic flow is considered as the sum of car behaviors as particles.
A microscopic model is suitable for high-resolution simulations where vehicle properties are heterogeneous, or flow characteristics vary from lane to lane, etc. However, they are computationally expensive since detailed vehicle behaviors must be updated at short intervals. On the other hand, a macroscopic model is computationally inexpensive and suitable to simulate large-scale traffic flow. However, it cannot capture individual car behavior. In a dynamic hybrid model, the application domains of micro- and macroscopic models can be switched during the simulation to achieve overall speed-up while keeping a high resolution of the area of interest.
The contribution to the research field is to model traffic flow phenomena at multiple resolutions and to propose methods to combine them. This presentation reports the results of improving the dynamic hybrid model already proposed by the authors. The model is also applied to an expressway merge section to evaluate its accuracy and computational efficiency.

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Recent advances in meshfree and particle methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COORDINATE TRANSFORMATION BASED ON SPH(2) FOR EFFICIENT FREE SURFACE FLOW SIMULATION

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ABSTRACT

The original SPH with fixed kernel functions guarantees accuracy in interpolation and numerical differentiation, only when particles are regularly and uniformly distributed. Therefore, the modified gradient operators are often used, where the first-order accuracy is preserved even when the particles are randomly distributed. On the other hand, there have not been much discussion on second-order derivatives (including Laplacian operators) and gradient models with higher-order accuracy. Hence, we proposed a class of SPH model, which we refer as "SPH(2)" [1], that satisfies second-order accuracy for both first- and second-order derivatives.

In this study, we utilize the SPH(2) for coordinate transformations that require first- and second-order derivatives including cross-derivatives. These transformations may help to reduce the heavy computations of particle methods, for example, in coastal engineering applications. We intend to develop to a "sigma-coordinate system", which changes the vertical resolution depending on the ocean depth, at the end, and as a first step, we generalize the vertical coordinate transformation in this study. The coordinate transformations for the ellipsoidal particle model [2] and the bottom boundary-fitted particle method [3] were performed using the SPH(2) operators to demonstrate the effectiveness of the proposed method.

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Scientific machine learning for geophysical applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EARLY FORECASTING OF TSUNAMI WAVEFORM WITH BAYESIAN SCENARIO-SUPERPOSITION

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ABSTRACT

Early tsunami warning plays an important role in disaster mitigation, and various methods that can forecast tsunami waveforms and/or inundation have been developed. Based on the lesson learned from past devastating tsunami events (e.g., the 2011 Tohoku tsunami event), researches have focused on improving the accuracy and immediacy of tsunami forecasting. In addition to such efforts, a probabilistic forecasting model will prevent under/overestimation of arrival wave heights since it can simultaneously provide prediction reliability. According to this background, we have proposed the early tsunami forecasting method based on the Bayesian theorem (Nomura et al., 2022). However, since the previous method only detects the “best-fit scenario” from a precomputed database by comparing the true waveforms, it cannot provide an accurate prediction if similar scenarios are not included in the database.

This study proposes an improved early tsunami forecasting method by introducing the scenario superposition concept based on the Bayesian theorem. This time, we focus on the Shikoku region (Japan) as a target site, which is threatened by the tsunami triggered by the Nankai Trough subduction zone. By GeoClaw software (Clawpack Development Team, 2021), we generate both training and test data consisting of synthetic tsunami wave heights. The test data is then input as an unknown tsunami event in the Bayesian technique which sequentially estimates/updates each training data-specific weight. Based on the evaluated weights, the scenario superposition is achieved by a linear combination of each hypothetical scenario in the precomputed database. It can be said that the present method is superior to the previous one because waveforms that have a much larger/smaller amplitude than all the trained scenarios, is predicted by not only interpolation but also extrapolation. Additionally, a probability distribution for the weight parameters is simultaneously obtained, which enables quantifying and visualizing the prediction reliability. We use the proposed and previous methods to forecast waveforms of test data and compare their results. Consequently, it was found that the proposed method could accurately predict waveforms, which could not be predicted by the previous method, within a 10-minute observation duration.

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THE METHOD OF FUNDAMENTAL SOLUTIONS USING ADAPTIVE SOURCE POINT SELECTION FOR TWO-DIMENSIONAL ELASTIC WAVE ANALYSIS

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ABSTRACT

The method of fundamental solutions (MFS) [1] is a numerical simulation method of mesh-free type and widely used for solving problems related to elastic deformation, vibration, and wave propagation. MFS uses fundamental solutions as a basis function and its approximate solutions are expressed by the linear combination of these fundamental solutions and approximation coefficients. In MFS, the source points of fundamental solutions are placed at arbitrary positions in the complementary domain of analysis one.

Compared with finite difference method (FDM) and finite element method (FEM), MFS requires fewer unknowns, because it does not require mesh generation of analysis domains and boundaries. Moreover, the numerical implementation of the MFS is simpler than that of boundary element method (BEM), because MFS can avoid the singular integration over the boundary. However, the accuracy of MFS is affected by the location of the source points. Thus, making the selection of suitable source point locations is a crucial task.

In this study, we develop a MFS which includes adaptive source point selection using orthogonal matching pursuit (OMP) [2]. OMP, a sparse modeling technique, can select appropriate basis functions from underdetermined system of equations. In our proposed method, we prepare source points whose number is more than that of equations and select adequate source points using OMP. We solve two-dimensional elastic wave problems using our proposed MFS and discuss its advantages and disadvantages.

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New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION FOR ADDITIVE MANUFACTURING UTILIZING IMAGE PROCESSING TECHNIQUES

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ABSTRACT

With the drastic development of additive manufacturing technologies in recent years, the high manufacturability of these techniques has garnered attention for enabling topology optimization with high design flexibility. However, when performing additive layer manufacturing, constraints such as overhang limitations, minimum thickness, and curvature exist, making it challenging to generate structures obtained directly from topology optimization calculations.
Focusing on overhang constraints, various methods have been proposed to reduce support material or aim for support-free structures[1-3]. Among these, approaches have been suggested considering the gradient of design variables, extracting angles from it, and applying constraints, as well as those leveraging the characteristics of mesh.
This study proposes a novel approach to consider constraints by developing a topology optimization design method based on image processing techniques. The angle information is extracted using the Sobel Filter, a form of image processing technology. Penalties are imposed on surfaces that do not satisfy stackable angles, and an objective function is defined to minimize these penalties. We formulate the multi-objective optimization problem, considering both stiffness and manufacturability.
We have successfully obtained optimized structures with higher performance and manufacturability by introducing this optimization problem as a post-process of conventional topology optimization problems. This paper presents numerical examples to demonstrate the validity and effectiveness of the proposed methodology.

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Architected materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STUDY ON THE MECHANICAL ASYMMETRY OF A NON-RECIPROCAL GEL USING COMPUTATIONAL HOMOGENIZATION

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ABSTRACT

Recently, mechanical asymmetry triggered by a specific loading direction has received attractive attention in the solid mechanics community. Materials exhibiting this asymmetry are expected to promote the development of asymmetric systems such as energy harvesting and material transport. A non-reciprocal gel (NR gel) developed by Ishida et al.[1] is a hydrogel containing magnetically oriented metal nanosheets, which can be regarded as a homogeneous material. The compressive load induces the buckling of nanosheets and results in the asymmetry of the macroscopic elastic response – the elastic modulus in the tensile direction is ten times larger than that in the compressive direction. Understanding the relationship between mechanical asymmetry and nanosheet buckling will facilitate the design of NR gels, leading to their application in various engineering fields.
In this study, we investigate influential factors that characterize the relationship between mechanical asymmetry and nanosheet buckling. The unit cell of NR gel is modeled as an elastic bilayer consisting of hydrogel and nanosheet, whose Young's modulus ratio and thickness ratio are parameterized. In the eigenvalue buckling analysis, the energetically preferred wavelengths for nanosheet buckling are computed for each parameter. The microscopic responses of NR gel are analyzed by the post-buckling analysis for the unit cell with the preferred wavelength and converted to macroscopic responses by the computational homogenization. We show that the microscopic responses are in good agreement with the analytical solution for layered composites[2]. We also find that the mechanical asymmetry of the macroscopic responses is pronounced as the Young’s modulus ratio increases or the thickness ratio decreases. We further analyze the in-plane spacing between nanosheets, which may also contribute to the mechanical asymmetry of a NR gel.

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Advanced computational modelling of wood, wood-based products, bio-composites, and timber structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADVANCED MULTISCALE MODELLING OF PLANT FIBER-REINFORCED BIOCOMPOSITES: BRIDGING THE GAP IN PREDICTIVE ANALYSIS FOR SUSTAINABLE CONSTRUCTION MATERIALS

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ABSTRACT

This study presents a novel approach in the predictive modelling of plant fibre-reinforced biocomposites, a sustainable and cost-effective alternative to conventional building materials. Biocomposites, consisting of natural cellulose fibres bonded with low CO2 footprint polymers like lignin [1], offer significant environmental advantages. However, their complex microstructure, characterised by variable fibre types, lengths, orientations, and mechanical interactions with the polymer matrix, has historically limited their use in load-bearing structural elements.

Our research addresses these challenges by developing advanced micromechanics-based multiscale modelling tools. These tools facilitate the comprehensive characterisation of 3D stiffness and, to some extent, the strength of natural fibres and their composites [2]. At the microscale, we consider various fibre orientations and aspect ratios, effectively representing biocomposite microstructures with diverse fibre configurations. Additionally, we incorporate a spring-type interface model within the continuum micromechanics framework to account for the typically weak fiber-matrix bond. This multiscale model is validated through uniaxial tensile tests on various plant fibre composites, accurately predicting the stiffness changes due to fibre alignment and interface compliance variations.

Furthermore, our approach employs nonlinear plasticity, XFEM, and cohesive zone models to simulate failure mechanisms, including matrix softening, fibre breakage, and fibre-matrix de-bonding, in a unit cell with periodic boundary conditions. This enables precise predictions of nonlinear macroscopic behaviour, validated against experimental data for both short- and long-fibre composites.

Our research paves the way for the practical application of lightweight biocomposite structures in real architectural contexts. The integration of these models with finite-element simulations and a 3D sketching tool provides a novel platform for material-informed computational design [3]. This study not only offers novel tools with respect to modelling and simulation of biocomposites but also contributes to the broader goal of developing sustainable construction materials.

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Advances in multi-scale, multi-material, and multi-component Topology Optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADVANCING STRUCTURAL SAFETY THROUGH INTEGRATED YIELD AND BUCKLING INDICATOR OPTIMIZATION

Christoffer Fyllgraf Christensen[*1], Fengwen Wang[1], Jonas Engqvist[2], Ole Sigmund[1] and Mathias Wallin[2]*

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ABSTRACT

This study addresses the challenge of identifying and preventing failure in engineering structures by combining yield stress and buckling indicators in topology optimization to enhance structural integrity and safety. Our approach integrates two key aspects: the inclusion of yield stress limits derived from homogenization-based analysis and the implementation of predictive buckling indicators within the structural design. Employing a novel framework, we incorporate local yield-based stress constraints based on a density-dependent von Mises yield surface alongside global and local buckling criteria. This methodology ensures that the resulting designs adhere to critical material yield behaviors crucial for practical applications. Additionally, our study embeds buckling indicators in the multiscale designs. Based on an adapted Willam-Warnke stress criterion presented by Christensen et al. [1], these indicators are engineered to visibly exhibit non-critical local buckling under load conditions just below global critical buckling. Inspired by the work of da Silva et al. [2], the blueprint design and a variant, where the predetermined indicator region is omitted, are considered. The result is an innovative safety feature, signaling the need for load reduction or maintenance. Experimental testing validates the correlation between the numerical simulations and the physical behavior of the printed structures, confirming the feasibility of our approach. Our research bridges the gap between theoretical optimization models and practical applications. By combining yield stress considerations and buckling indicators, we not only ensure adherence to material and mechanical performance but also introduce a novel safety paradigm in engineering design. The integrated approach contributes significantly to structural safety, offering built-in early-warning failure prediction capabilities and paving the way for more reliable and safer structural implementations.

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Modeling and simulation of advanced manufacturing processes for metals
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEM SIMULATION TO PREDICT THE POWDER BED QUALITY FOR ADDITIVE MANUFACTURING PROCESSES.

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ABSTRACT

Many metal additive manufacturing (AM) technologies, such as laser powder bed fusion (LPBF), rely on the stacking of thin powder layers with a rigid blade or a roller. The spreading step is critical because defects in the powder bed (i.e., low packing density, poor surface uniformity, particle segregation, etc.) often result in defects in the final product (i.e., lack of fusion, porosity, etc.). Currently, the lack of understanding of the spreading process, which depends, among other factors, on the powder properties and spreader geometry, results in a trial-and-error approach to ensure a quality powder bed which is not cost effective. Discrete Element Method (DEM) simulations can help us understand the mechanisms at play during the spreading process and select the best operating parameters (i.e., spreader geometry, spreader speed, layer thickness, etc.) for a given powder feedstock.

In this work, we first present Lethe, an open-source DEM software capable of simulating the spreading of multiple powder layers, with periodically moving spreaders, powder dispenser platform and build-plate, all in a single simulation. We then use this software to run large-scale DEM simulations, evaluating the influence of the operation parameters and of the DEM parameters related to the feedstock (i.e., surface energy, restitution coefficient, friction coefficients, etc.) on the powder bed quality. Finally, through a collaboration with the National Research Council of Canada, we use an experimental set-up that replicates the whole spreading process while allowing freedom on operating parameters. This experimental set-up measures the relative density of the powder bed in between each layer. Using DEM simulation, we replicate these experimental results to assess the role of the powder property on the bed density and to gain insight into the physical mechanism affecting the bed quality in certain operating conditions. This paves the way for a digital twin for powder spreading that could swiftly identify powder bed quality from the powder property and the operating parameters.

Space-time modeling of coupled problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VARATIONAL PRINCIPLES FOR COUPLED CHEMO-MECHANICS IN ELASTIC AND DISSIPATIVE SOLIDS

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ABSTRACT

Variational principles for coupled chemo-mechanical problems in elastic and dissipative solids at infinitesimal strains are outlined in the present work. In doing so, it is seen that the gradient of the primary fields additionally enter the energetic and dissipative potential functions, resulting in additional balance equations. The governing balance equations of the coupled problem are derived as Euler equations of the incremental variational principles, formulated in continuous-and discrete-time/space settings. Furthermore, the variables governing the inelastic process are locally condensed which yields a reduced global problem that is solved in a discrete-space-time setting. The symmetric structure of the proposed framework with respect to the primary and state variables is an advantage, and this is exploited in the numerical treatment within the finite element paradigm. The framework is applied to Cahn-Hilliard- type diffusion and Allen-Cahn-type phase transformation in elastic and dissipative solids. The applicability of the proposed framework is demonstrated by means of two- and three-dimensional representative numerical simulations.

Battery modeling and computation: From material to device
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DENDRITE INHIBITION STRATEGY USING HETERO-EPITAXIAL RESIDUAL STRESSES IN THIN FILM DEPOSITION MECHANICS

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ABSTRACT

Dendrite formation is a long-standing problem for the commercial application of rechargeable metal anode batteries. The well-controlled coating on anodes can solve the problem of instability and uncontrolled reactions between electrodes and electrolytes. Understanding the effects of pre-stressed (residual stress) electrodes with artificial solid-electrolyte inter-phase layer (thin film) on dendrite formation is crucial for the successful application of stable anodes. In this work, using DFT-informed continuum modeling and phase-field modeling, we studied the impacts of residual stresses on the surface evolution of atomic/molecular layer deposited (ALD/MLD) Al2O3 and alucone coating on Zn anodes. During the thin film deposition process, the induced stress arises from two sources, namely, the residual stress during fabrication and the mechanical stress associated with the volume expansion. Of the two, residual stress has largely been considered to have a negligible effect without any rigorous evidence being put forward. Epitaxial stresses are one of the major sources of residual stress in the hetero-epitaxial thin films, which are sensitive to the misfit in crystal lattices existing between film and substrate. The epitaxial stresses influence defect formation in most thin-film systems. We critically assessed alucone and alumina-coated Zn surfaces to depict a prospective methodology to reduce the dendrite growth using the developed hetero-epitaxial residual stress. We used DFT-informed misfit strain analysis in the phase field model to understand the significant consequences of residual stress, such as microstructural changes and deformation in the materials.

Advanced numerical techniques for fluid flow in porous media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL SIMULATION OF THE 2-D COMPOSITIONAL FLUID FLOW MODEL IN HETEROGENEOUS AND ANISOTROPIC PETROLEUM RESERVOIRS USING A MULTIPOINT FLUX APPROXIMATION FINITE VOLUME WITH A DIAMOND STENCIL (MPFA-D) COUPLED TO A HIGH ORDER MUSCL-TYPE SCHEME

Maria Galindo[*1], Darlan Carvalho[1], Paulo Lyra[1] and João Andrade[1]*

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ABSTRACT

The use of the compositional reservoir simulation has become an important tool to accurately predict the oil and gas recovery in complex petroleum reservoirs, and in the modelling of complex phenomena such the enhanced oil recovery processes. Although the compositional model based on Equations of State (EOS) produces a much better description of the fluid flow behavior when compared with the simpler “black oil” model, its use can be very computationally demanding, due to the solution of a large system of Partial Differential Equations (PDEs) composed by the component mass conservation, Darcy’s low and the fugacity constraints. Besides, to properly model the fluid flow in geologic complex heterogeneous and anisotropic reservoirs including “Y” faults and pinchouts and to properly represent inclined wells the use of unstructured computational meshes can be of utmost importance. In this context, to solve the system of PDEs we have used the classical IMPEC (Implicit Pressure Explicit Composition) strategy along with the Peng-Robinson’s Equation of State to model the phase behavior during the fluid flow in the reservoir. To approximate the pressure equation, we have used the Multipoint Flux Approximation with a Diamond Stencil (MPFA-D) finite volume method and the second order Monotone Upstream-centered Scheme for Conservation Laws (MUSCL) for the solution of the component transport equations along with an adequate multidimensional limiting strategy to suppress spurious numerical oscillations. For the time integration we have used the third order Runge–Kutta method. To evaluate our formulation, we have solved some benchmark problems found in literature with very promising results when compared to other classical schemes particularly for problems involving unstructured and non k-orthogonal meshes and full tensor rock permeabilities.

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Innovations in machine learning-enhanced uncertainty quantification for computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SIMULATION-BASED INFERENCE OF DYNAMICAL SYSTEMS WITH MODEL UNCERTAINTY

Nick Galioto[*1] and Alex Gorodetsky*[1]

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ABSTRACT

Accounting for model uncertainty during the estimation of dynamical systems is important for generating reliable and generalizable predictions. For state-space systems, quantification of model uncertainty can be achieved through the estimation of an added process noise term in the system dynamics [1]. Within a Bayesian framework, the inclusion of process noise in the model formulation has shown to improve the likelihood smoothness and yield inherent regularization during estimation [2]. The cost of adding process noise, however, is that the system states become uncertain and must be marginalized out when evaluating the likelihood, requiring costly integration. The cost can be mitigated with recursive filtering algorithms, but these algorithms require inversion of covariance matrices, resulting in a computational complexity that scales cubically with the state and measurement dimensions. As a result, the filtering algorithm is unsuitable for even moderate dimensions.

Simulation-based inference (SBI) methods offer an alternative means for constructing an approximate likelihood at a potentially lower computational cost. These methods circumvent the challenge of computing costly or intractable likelihoods by using outputs from a model simulator to estimate a surrogate density function that can be evaluated efficiently, e.g., a neural network. In this talk, we consider two SBI methods for likelihood approximation: the sequential neural likelihood and the Bayesian synthetic likelihood. We present the advantages and disadvantages of each approach in comparison to the filtering-based approximation and discuss the feasibility of extending each algorithm to problem settings with model uncertainty. Then, we benchmark each algorithm on noisy, single-trajectory data from the Lotka-Volterra predator-prey model. In this comparison, we analyze the differences in cost and effective sample size between the methods for posterior sampling.

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Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

REDUCED-ORDER PHASE-FIELD MODELING FOR CONTROLLED MICROSTRUCTURE IN ADDITIVE MANUFACTURING

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ABSTRACT

One of the significant challenges associated with Laser Powder Bed Fusion (L-PBF) is the evolution of microstructures (i.e., crystalline grain structures), which has a significant impact on the final material properties. To address this challenge, our study presents a physics-guided and machine-learning-aided approach for optimizing scan paths to achieve the desired microstructure outcomes, particularly focusing on the generation of equiaxed grains which are desirable for enhanced material properties. We utilize phase-field (PF) modeling, a physics-based computational method, to gain insights into microstructure evolution. The high computational costs associated with PF modeling can be mitigated by employing machine learning reduced-order or surrogate models. We will introduce two approaches for accelerating phase field models. The first one is a physics-embedded graph network, which leverages an elegant graph representation of the grain structure and embed the classic PF theory (e.g., Allen-Cahn equation) into the graph network. The second approach is by training a surrogate machine-learning model using a three-dimensional (3D) U-Net convolutional neural network. This approach enables the learning of microstructure evolution in a supervised manner, with the machine learning model being able to predict crystalline grain orientations with high accuracy based on the initial microstructure and thermal history. The training data pivotal for our machine-learning model is generated from single-track, single-layer PF simulations, under various process parameters. We aim to capture the essential characteristics of grain structures in a compact representation. The developed approach effectively minimizes computational demands, yielding a structured and accessible search space for optimization. Leveraging the reduced-order models, we implement a reinforcement learning strategy, finely tuning the laser tool path to precisely attain the desire crystalline microstructure.

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Machine learning and data driven based engineering computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADVANCING THE DESIGN OF COMBINED PILED-RAFT FOUNDATIONS: AN INTEGRATED APPROACH OF SUPERVISED MACHINE LEARNING AND ANALYTICAL METHODS

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ABSTRACT

The Combined Piled-Raft Foundation (CPRF) is recognized as a highly economical and effective foundation system for towering structures. However, its intricate design process is often marked by time-intensive challenges. Addressing this, several closed-form approximate solutions have been proposed in the past. Nonetheless, the reliability of these solutions, particularly for preliminary design stages, remains a topic of debate.

In this study, we rigorously evaluate the applicability and accuracy of three prevalent approximate solutions in the analysis of CPRF systems. These methods include the Poulos-David-Randolph method (PDR), the equivalent pier method (EP), and the equivalent raft method (ER). Our evaluation is grounded in a comparative analysis with a benchmark 3D finite element model. This comprehensive assessment involved 700 cases across varying CPRF configurations, encompassing 20 distinct dimensional parameters such as pile length, diameter, spacing, as well as the width and length of the raft.

The crux of our study lies in the application of supervised machine learning techniques. These advanced methodologies were employed to ascertain the validity domain of each evaluated method. The primary objective was to delineate the specific conditions under which each method can be applied with utmost accuracy. Our findings aim to streamline the design process of CPRFs, thereby enhancing both the efficiency and the reliability of foundation designs for tall buildings. This study stands at the intersection of traditional analytical approaches and cutting-edge machine learning applications, heralding a new paradigm in engineering practices.

Multi-scale, multi-rate damage and fracture: Models, experiments, and simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFECTS OF VOID SHAPE AND DISTRIBUTION ON DUCTILE FRACTURE BASED ON UNIT-CELL CALCULATIONS

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ABSTRACT

Ductile fracture in porous metallic materials is primarily governed by void behavior according to the previous studies. In this study, we explore the effect of initial void shape and distribution on ductile failure under various stress states based on unit-cell calculations. The credibility of our numerical findings is validated through mechanical tests conducted on additively manufactured specimens.
A proportional loading is applied on the unit cell to matin a constant loading state during the deformation. Different criterions are employed to identify the strain localization and void coalescence behavior [1]. Spherical, oblate, and prolate voids serve are employed as the initial shapes for single-voided unit cells, allowing us to identify void growth, strain localization, and void coalescence varying stress triaxialities. Additionally, we also investigate the effect of void distribution effect on ductile fracture with multiple regularly or randomly distributed voids.
Our numerical results show that the geometric asymmetry resulting from the initial void shape induces anisotropic deformation and failure. Strain localization for the spherical void occurs earlier than for other void shapes at high stress triaxiality, instead of occurring between the prolate void and the oblate void for void coalescence. A greater thickness enhances deformation capacity and delay void coalescence under high stress triaxiality. The conclusion also corroborated by calculations through multiple-voided unit cells. Furthermore, simulations of multiple-voided unit cells reveal that ductile fracture can be influenced by adjusting void distributions and loading conditions. Void clusters may promote the fracture occurrences, even as the initial void fraction decreases. Controlling the main loading direction on components emerges as a strategy to govern fracture behavior through adjusting defect distribution.

Our numerical findings offer valuable insights into specific mechanical and tomographic experiments involving additively manufactured components [2]. Additionally, our investigation illustrates on the potential for manufacturing more fracture-resistant components through additive manufacturing, underscoring the significance of defect engineering in metallic material fracture control.

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Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMPLEMENTATION OF EXTRINSIC COHESIVE ZONE MODEL (ECZM) IN 2D FINITE-DISCRETE ELEMENT METHOD (FDEM) USING NODE BINDING SCHEME

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ABSTRACT

The combined finite-discrete element method (FDEM) has been widely used for rock fracturing simulations. Conventionally, FDEM is realized using the intrinsic cohesive zone model (ICZM); however, it has the drawback of artificial compliance and high computational expense. As a complement, the extrinsic cohesive zone model (ECZM) is seen to be realized in FDEM recently, whereas the node splitting scheme utilized is cumbersome. Here, within the framework of ICZM-based FDEM, we propose a node binding scheme to efficiently bind the pre-discretized finite elements and thus guarantee the continuum behavior of materials in the elastic stage. The yield surfaces, controlled by ECZM, are dynamically embedded by invoking the pre-inserted cohesive elements. The effectiveness and efficiency of the proposed approach are validated and tested by performing a suite of numerical experiments. Compared with ICZM-based FDEM, the proposed approach can correctly capture material deformation and reduce the computation cost. In contrast to the existing ECZM-based FDEM, the proposed approach can overcome the frequent and complex element topology updating. This work provides a novel perspective that fully inherits the advantages of both ICZM and ECZM, but circumvents their shortcomings, which guarantees a more efficient and effective simulation of brittle material evolution from continuum to discontinuum.

Design and mechanics of mutifunctional composites and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION METHOD OF SKIN-TO-SKELETON CONNECTION AREA'S DISTRIBUTION DESIGN FOR ALLEVIATING STRAIN CONCENTRATION AND SUPPRESSING WRINKLES OF FLEXIBLE SHEETS

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ABSTRACT

Morphing wing can get over the limitation of traditional aircraft's fixed shape and achieve the best aerodynamic efficiency. However, the phenomenon of excessive strain in local area of flexible skin surface and skin bump due to aerodynamic loads frequently occurs in the morphing process of wings. How to alleviate strain concentration of the skin and suppress skin wrinkles are crucial considerations in the morphing process of the flexible sheet. In this paper, we propose a strategy to improve the uniformity of the strain distribution and suppress skin wrinkles through rationally distributing the connection areas between the skin and skeleton of the sandwich-flexible-sheet, and develop a topology optimization method for determining the optimal distribution of the connection areas. In this method, the connection areas between the skin and the support skeleton are considered as the virtual adhesion layer comprising of adhesion materials. Based on the topology optimization idea, the distribution of connection areas is described by allocating the presence and absence of the adhesion material. The optimization model is established with minimizing the globe stress of the skin as the objective function, the volume fraction of the design domain and the normal deflection of the maximum displacement points in the skin wrinkles areas as constraints. The effectiveness of the proposed method is verified through examples involving tensile and rotational states of the sandwich-flexible-sheet with Ω-shaped honeycomb skeleton structure, and the results show that the optimization method can significantly improve the strain distribution of the skin and mitigate the degree of wrinkles. Finally, a variable-sweep structure for unmanned aerial vehicles (UAVs) is designed to explore the practical value of the proposed method.

A FINITE ELEMENT-INSPIRED HYPERGRAPH NEURAL NETWORK: APPLICATION TO FLUID FLOW AND FLUID-STRUCTURE INTERACTION SIMULATIONS

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ABSTRACT

An emerging trend in deep learning research focuses on the applications of graph neural networks (GNNs) for mesh-based continuum mechanics simulations. Most of these learning frameworks operate on graphs wherein each edge connects two nodes. Inspired by the data connectivity in the finite element method, we present a method to construct a hypergraph by connecting the nodes by elements rather than edges. A hypergraph message-passing network is defined on such a node-element hypergraph that mimics the calculation process of local stiffness matrices. We term this method a finite element-inspired hypergraph neural network, in short FEIH(phi)-GNN. We further equip the proposed network with rotation equivariance, and explore its capability for modeling unsteady fluid flow systems. The effectiveness of the network is demonstrated on flow around bluff and streamlined bodies. Stabilized and accurate temporal roll-out predictions can be obtained within the interpolation Reynolds number range. The network is also able to extrapolate moderately towards a higher Reynolds number domain out of the training range. Adopting the arbitrary Lagrangian-Eulerian formulation, we further construct a quasi-monolithic framework that enables the modeling of fluid-structure systems, and applied such a framework to two prototypical cases, namely the flow around an elastically mounted cylinder, and the flow around a hyperelastic plate attached to a fixed cylinder. The proposed framework tracks the interface description and provides stable and accurate system state predictions during roll-out.

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Computation for energy storage
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INTEGRATING MECHANICS, PIEZOELECTRICITY AND ELECTROCHEMISTRY

Tianhan Gao[1] and Wei Lu*[1]

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ABSTRACT

Lithium metal battery provides the highest possible theoretical capacity. However, one of the biggest challenge in realizing lithium metal battery is dendrite growth during lithium deposition, which leads to internal short circuit and safety hazard when it pierces through the separator. Dendrite penetration is also the key barrier for achieving fast charging in current lithium ion batteries. We show a new mechanism of stopping dendrite formation by using the mechanical deformation of a piezoelectric film or coating. A local over-potential appears when a piezoelectric separator film is deformed by any surface protrusion. This piezoelectric over-potential reduces the driving force of lithium diffusion toward any protrusion, resulting in a flat lithium metal surface. We developed a computational framework that integrates mechanics, piezoelectricity and electrochemistry [1-3]. With this framework, we have investigated the electrodeposition of lithium ions on a lithium metal surface through a porous piezoelectric film. Simulations show how dendrites forms and grows during regular lithium ion deposition, while a piezoelectric film completely stops any dendrite nucleation.

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Battery modeling and computation: From material to device
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMPEDANCE INHOMOGENEITY INDUCED BY THE SIO ADDITION IN SIO/GR COMPOSITE ANODE

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ABSTRACT

Silicon/Carbon (Si/C) composite anode materials have emerged as promising candidates for high-energy-density lithium-ion batteries (LIBs), boasting advantages such as high capacity, cost-effectiveness, and abundance. However, the integration of Si-based materials into conventional C anodes introduces heterogeneous interactions between electrochemical and mechanical behaviors, owing to substantial volume changes and chemical potential variations. One significant consequence of these interactions is the impedance inhomogeneity, which adversely affects the discharging capacity of Si-based LIBs. In an effort to comprehensively understand this phenomenon and its underlying mechanisms, an electrochemo-mechanical coupled model is established, incorporating detailed particle geometries on the anode side. The model is employed to investigate polarization components and their evolution during the charging/discharging process. Various influencing factors, such as SiO weight percentage (wt.%), electrode thickness, and SiO distributions (both in terms of distribution uniformity and direction), are systematically discussed. This study offers an efficient computational approach to analyze battery polarizations, deepening the understanding of the inhomogeneous evolution of these polarizations in Si/C composite anodes. Ultimately, these insights guide the design of anodes for next-generation high-energy-density LIBs.

Modeling and simulation of advanced manufacturing processes for metals
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EVOLUTION OF MICROSTRUCTURE GRAINS IN THREE-DIMENSIONAL PHASE FIELD DURING WIRE ARC ADDITIVE MANUFACTURING PROCESS

Xiang Gao[*1] and Zhao Zhang*[1]

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ABSTRACT

In the WAAM process, the growth and evolution of grains are affected by the morphology of the melt pool, and the microstructure of the components are influenced by the growth of grains and the evolution between columnar and equiaxed grains significantly. Based on the double ellipsoidal heat source, the morphology of the melt pool under different heat source parameters was studied. A three-dimensional phase field model containing a heterogeneous nucleation model was developed to study the microstructure evolution under different process conditions in the WAAM process. The results indicate that the depth of the molten pool increases with the increasing of arc power and the decreasing of arc scanning speed. The size and growth direction of grains are mainly controlled by the morphology of the melt pool. The interior and top of the component are composed of columnar grains and equiaxed grains, respectively. With the unidirectional travel direction deposition strategy, the bending degree of columnar grains increases with the decreasing of arc scanning speed. The increasing of arc power and the decreasing of speed lead to grain coarsening. With the bidirectional travel direction deposition strategy, the growth direction of columnar grains changes, resulting in the formation of bent columnar grains.

Recent advances in computational fracture mechanics and failure analysis
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE MODELING OF HYDROGEN TRANSPORT IN STEELS AND ITS RESULTING EMBRITTLEMENT EFFECT

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ABSTRACT

A multiscale modeling approach is adopted in this study to understand the hydrogen embrittlement (HE) mechanisms and to predict failure of engineering components subjected to complex stress state and under the influence of hydrogen environment. Firstly, molecular dynamics simulations of the body-centered cubic (BCC) iron are conducted on an atomistic scale to examine the effect of hydrogen on the fracture behavior with the focus on the influence of grain boundaries (GB). An increase in dislocation nucleation at the crack tip region due to the presence of hydrogen contributes to the so-called hydrogen enhanced localized plasticity (HELP). It is observed that change in atomic structure leads to localized dislocation pile ups and void formations, which facilitates fracture and embrittles the material. Various GB types and orientations as well as mixed mode loadings are considered to assess the impact of grain boundary energy and mode mixity on the hydrogen effect on crack propagation. Next, the effect of stress state on ductile failure under the influence of hydrogen is studied at the microscale by incorporating the hydrogen diffusion process and the HELP effect into a finite element program and performing a series unit cell analysis. It is shown that localized plastic deformation plays a major role in increasing the local hydrogen concentration due to the newly generated trapping sites and the HELP effect promotes material failure by accelerating void growth. The fracture process is strongly affected by the stress state subjected by the material unit characterized by the stress triaxiality and Lode parameter. Lastly, a numerical framework is developed at the macroscale by incorporating hydrogen transport in steels and the resulting HELP and HEDE (hydrogen enhanced decohesion) mechanisms into a phase field model to simulate hydrogen embrittlement and crack propagation in engineering components. The results show that both HELP and HEDE reduce the specimen’s load carrying capacity. With properly chosen model parameters, the numerical model can predict crack propagation and ductile to brittle transition due to the presence of hydrogen.

Advance and application of meshfree methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GENERALIZED WEAK-FORM FREE ELEMENT METHOD FOR SOLVING MECHANICS PROBLEMS

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ABSTRACT

In this study, two generalization methods are proposed for extending the Weak-form Free Element Method (WFrEM) to solve heat conduction, solid and fluid mechanics problems by using general iso-parametric elements with and without internal nodes. The first generalization is performed based on the interface force/flux equilibrium of all elements around the collocation point as done in FEM and the second one is fulfilled by setting up a control volume within a free element as done in FVM.
These generalizations can break through the restriction of FrEM on using elements having at least one internal node. Besides, the free element control volume method presented in this study can overcome the difficulty in FVM that high-order solution schemes cannot be easily formed.

In the generalized WFrEM, also called the extended WFrEM, the meshes used in the standard FEM as well as the polygon/polyhedron elements can also be naturally used.

Detailed formulations of the generalized WFrEM for solving heat and mechanics problems are given in the study and a number of numerical examples will be analyzed to verify the correctness and stability of the proposed method.

Keywords: Generalized weak-form free element method, Extended weak-form free element method, Free element control volume method, Free Element Method, Heat conduction, Mechanics.

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Applications of shape optimization in complex engineering problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DISCRETE ADJOINT METHOD ON DYNAMIC MESHES WITH LOCAL GRID TOPOLOGY MODIFICATION

Yisheng Gao[*1], Fei Qing[1], Jiajun Long[1], Ao Zhang[1], Shengguan Xu[2] and Jiale Zhang[3]*

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ABSTRACT

During the last three decades, the adjoint method has been widely used for aerodynamic design problems, since the calculation cost of the gradient for objective function is of the same order of magnitude of single flow solution, essentially independent of the number of design variables. For unsteady flow problems involving moving and deforming boundaries, the arbitrary Lagrangian Eulerian (ALE) formulation is particularly useful, as it combines the advantages of the Lagrangian and the Eulerian approaches and possibly reduces their drawbacks. And it can be easily combined with discrete adjoint method to solve unsteady aerodynamic optimization problems. However, if local modification of connectivity occurs, the discrete adjoint formulation is unavailable. In this paper, an accurate and efficient discrete adjoint method is presented for aerodynamic design optimization on three-dimensional dynamic meshes with local grid topology modification. The key issue here is the interpretation of local topology modification in the adjoint framework. An interpolation-free conservative ALE scheme, proposed by Guardone et al. [Arbitrary Lagrangian Eulerian formulation for two-dimensional flows, Journal of Computational Physics 230, (2011)], is applied to interpret the local topology modification as continuous deformation of the corresponding elements. Therefore, the discrete adjoint formulation can be naturally applied to these elements, analogous to the fixed-connectivity case. To avoid manual implementation of discrete adjoint, automatic differentiation (AD) is used to construct the duality-preserving discrete adjoint for the complete unsteady simulation. The advantages of the present method are as follows: (1) The present method can be used to arbitrary mesh movement or deformation, not only the case of small boundary displacement or the movement of multiple rigid bodies. (2) Most of the necessary terms in adjoint formulation are created by AD tool, so large part of discrete adjoint implementation is automatic and lengthy development time is avoided. (3) The adjoint formulation here is the exact adjoint of the tangent model, which is featured of exact duality preserving in the complete optimization problem. So the gradient of object function in adjoint model is perfect consistent with that obtained in tangent model or other exact numerical differentiation methods in machine precision. This feature also affords a convenient verification of discrete adjoint code. (4) Applying the AD tool selectively can dramatically improve the performance of AD based adjoint implementation, achieving similar efficiency to hand-coded version. Several three-dimensional design problems are presented to demonstrate the effectiveness of the proposed method.

A MECHANICAL-ELECTRIC COUPLING MODEL FOR SUPERCONDUCTING CORC CABLES

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ABSTRACT

The conductor on round core (CORC) cable is new type supercondcuting cable, which is one of the best candidates for the next generation nuclear fusion magnets due to its simple preparation process, high current carrying and low AC loss. CORC cable in the preparation and operation process will be affected by mechanical force, thermal and electromagnetic load, will produce axial tensile, transverse compression and torsion and other different deformation. Therefore, the analysis on the mechanic-electric behavior is the key link of cable design and preparation. In this study, a coupling mechanical-electromagnetic model is established for CORC cable, and the influence of mechanical strain on its critical current is considered. The behavior of critical current degradation and AC loss of CORC cable under different deformation modes is discussed. The effects of cable winding angle, types gap, and the material properties of the cable core structure on the mechanical-electric behavior of CORC cable are further parameterized studied, and some experimental phenomena are explained. All the results indicate that the model has a good prediction accuracy for different deformation mode. For example: for the torsion case: compared to the previous model, the error between the simulation results and the experiment is reduced from 46% to less than 10%.

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Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A FRACTURE MECHANICS-BASED APPROACH FOR CYLINDRICAL CAVITY EXPANSION IN THE ELASTOPLASTIC MEDIUM

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ABSTRACT

Cylindrical cavity expansion problems in the elastoplastic medium are common in geomechanics, including mining and petroleum engineering. The elastoplastic constitutive model is often used to analyze these problems, leading to a continuum solution. However, localized deformation caused by softening is generally observed in geomaterials, and hence the fracture mechanics-based method becomes an alternative approach to the problem.

In this approach, instead of assuming the existence of a plastic zone surrounding the cavity, a group of evenly distributed shear fractures initiates and propagates from the cavity boundary in the elastic medium. The Mohr-Coulomb criterion is enforced over the shear fractures to establish the relationship between the normal and shear stresses on the fracture surface. The minimum plastic dissipation criterion is adopted to determine the fracture propagation direction. The problem is discretized by the displacement discontinuity method, and then solved numerically by an optimization algorithm [1-3].

The numerical simulation solution converges to the traditional plastic constitutive model as the number of shear fractures increases, where the convex hull of the fracture tips is interpreted as the plastic zone. Additionally, the external loading and radial displacement over the cavity boundary also converge to the solution obtained by the traditional elastoplastic solution. This fracture mechanics-based approach provides us with a novel tool for investigating the softening and localization behavior of the elastoplastic medium.

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Constitutive modeling of complex materials with machine learning and artificial intelligence
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SYMMETRY-ENFORCING NEURAL NETWORKS FOR CONSTITUTIVE MODELING

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ABSTRACT

The use of machine learning techniques to homogenize the effective behavior of arbitrary microstructures has been shown to be not only efficient but also accurate. In a recent work, we demonstrated how to combine state-of-the-art micromechanical modeling and advanced machine learning techniques to homogenize complex microstructures exhibiting non-linear and history dependent behaviors [1]. The resulting homogenized model, termed smart constitutive law (SCL), enables the adoption of microstructurally informed constitutive laws into finite element solvers at a fraction of the computational cost required by traditional concurrent multiscale approaches. In this work, the capabilities of SCLs are expanded via the introduction of a novel methodology that enforces material symmetries at the neuron level, applicable across various neural network architectures. This approach utilizes tensor-based features in neural networks, facilitating the concise and accurate representation of symmetry-preserving operations, and is general enough to be extend to problems beyond constitutive modeling. Details on the construction of these tensor-based neural networks and their application in learning constitutive laws are presented for both elastic and inelastic materials. The superiority of this approach over traditional neural networks is demonstrated in scenarios with limited data and strong symmetries, through comprehensive testing on various materials, including isotropic neo-Hookean materials and tensegrity lattice metamaterials. This work is concluded by a discussion on the potential of this methodology to discover symmetry bases in materials and by an outline of future research directions.

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Physical models and reduced order models augmentation with data for physics-informed machine learning in real-world applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICS-INFORMED NEURAL NETWORKS FOR BLOOD FLOW INVERSE PROBLEMS

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ABSTRACT

Physics-informed neural networks (PINNs) [1] have emerged as a powerful tool for solving inverse problems, especially in cases where no complete information about the system is known and scatter measurements are available. This is especially useful in hemodynamics since the boundary information is often difficult to model, and high-quality blood flow measurements are generally hard to obtain. In this work, we use the PINNs methodology for estimating reduced-order model parameters such as the ones used in the Windkessel model [2], and the full velocity field from scatter 2D noisy measurements in the ascending aorta. The results show robust and accurate parameter estimations when using the method with simulated data, while the velocity reconstruction accuracy shows dependence on the measurement quality and the flow pattern complexity. In conclusion, the presented methodology allows for solving clinical-relevant inverse problems in hemodynamics and complex coupled physical systems.

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Advancing computational mechanics with symbolic regression
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A PHYSICS-INFORMED MACHINE LEARNING APPROACH TO MODELING THE CONSTITUTIVE RESPONSE OF A SINGLE CRYSTAL WITH VOIDS

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[3]University of Carolina, Santa Barbara

ABSTRACT

Modeling the coupled constitutive response and evolution of voids during plastic flow is critical for both component manufacturing and lifetime estimation purposes. To this end, we propose a new homogenized constitutive equation for modeling the stress-driven response of a rate-dependent, plastically anisotropic FCC single crystal with voids that deforms by plastic flow. The approach combines an analytically-based micromechanical component, which ensures theoretical consistency, with a data-driven symbolic regression component, which captures analytically intractable mechanisms. This hybrid approach also uses a systematic strategy to
identify problem-specific physics-informed solution requirements before conducting the data-driven component. The data-driven component consists of a physics-informed genetic programming-based symbolic regression (P-GPSR) algorithm that can exploit these solution requirements in conjunction with data. Here, the problem is contextualized as a multiform optimization problem in which the same set of data-driven components are embedded in a new gauge function and a new strain rate function. This contextualization helps mitigate potential overfitting and also expands the available training data to include both an effective stress measure and strain rate. This is also a multiobjective optimization problem, and the genetic algorithm benefits from a supplementary search and selection step that mitigates challenges satisfying competing objectives. Notably, the P-GPSR produced constitutive equations are theoretically consistent and the physical significance of all terms is known.

Towards predictive digital twins: Innovative algorithms for physics-, data-assisted and hybrid modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPRESSIVE STOCKING OPTIMIZATION FOR LYMPHEDEMA TREATMENT AT LOWER-LIMB

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ABSTRACT

The lymphatic system is the responsible to collect the lymph and return to the bloodstream. Lymphedema is disease that causes swelling in the body's tissues due to accumulation of lymph, which usually takes places in the extremities. It may occur due to genetic reasons or as a result of damage to the lymphatic system, such as after cancer treatment. This research focuses on the treatment of lymphedema at lower-limb through compression stockings, which is a widely applied measure to reduce the volume of edemas [1].

Despite effective at a clinical level, the use of off-the-shelf stockings with predefined sizes, reduces the efficiency. With the long-term aim of designing patient-specific stockings, this study aims to develop real-time simulation tool to predict the most suitable stocking for a given patient. For such purpose, the use of standard Finite Element techniques falls short, as large models are needed which implies high computational cost.

For this purpose, a solution based on Reduced Order Model (ROM) is developed to compute, in real-time, the tissue hydrostatic stress distribution at the location of the lymphatic system [2]. Hydrostatic stress is a compressing pressure that squeeze lymphatic vessels (hypertension), which improves lymph circulation and increase the drainage capacity.

Starting from CT-scan of patients, the geometry is registered through a reduced number of parameters applying Free-Form Deformation algorithm. These parameters are the inputs of the ROM together with material properties. The ROM requires to solve a high number of FE models defined through the mentioned parameters to create a training dataset. Such pre-processing step is carried out through Gridap [3], an open source finite element method library written in Julia.

This method enables to design the most efficient compressive stockings considering the particularities of each patient, which improves the drainage of lymph at lower-limb. It provides the required compressive pressure applied by the stocking which is an important fact to design the patient-specific stockings.

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New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ROTOR-STATOR DESIGN TO TRANSPORT COMPRESSIBLE TURBULENT FLOW UNDER THE TOPOLOGY OPTIMIZATION METHOD

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ABSTRACT

The energy consumed by a compressor heavily depends on the design of the rotor-stator coupling. Both components play distinct roles: the rotor for compression and the stator for directing the flow. Simultaneous analysis of both components is required to avoid miscalculations arising from aerodynamic effects, such as tip vortexes [1]. The interaction between the rotor and stator in fluid leads to pressure fluctuations and is imperative to comprehensively characterize and control these fluid excitations, which are compressible due to rapid changes in flow density, direction, and velocity. Therefore, the current research develops a rotor-stator design considering the flexibility of the topology optimization method, which has shown efficient and innovative designs for the transport of incompressible flow at rotor-stator systems [2]. This research novelty relies in the transport of compressible turbulent steady-state flow under a multi-reference frame domain that separates the rotating part from the stator section. The primal state equations are solved using the rhoSimpleFoam solver from OpenFoam, and the adjoint system is solved using automatic differentiation from FENICS (dolfin-adjoint) [3]. The IPOPT optimizer is used, and a material density-based distribution is employed to define the permeability of the cell's domain. The method is validated through a sensitivity analysis, and 2D rotors-stator couplings are optimized under different rotations, showing the importance of optimizing both systems under a multi-reference frame approach successfully.

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Advanced model order reduction techniques for computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ENHANCING FLUID MECHANICS ANALYSIS: APPLYING ORDER-TRUNCATED IMAGINARY ALGEBRA FOR EFFICIENT SENSITIVITY ANALYSIS IN FLUID SIMULATIONS

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ABSTRACT

Sensitivity analysis in fluid mechanics plays a critical role in understanding and predicting how changes in specific parameters or conditions affect the behavior of fluid flow systems. Fluid mechanics, with its inherent complexity due to the behavior of fluids under various conditions, benefits greatly from such analysis.
Sensitivity analysis is used to understand fluid behavior: fluid systems can be susceptible to parameter changes like velocity, pressure, temperature, and viscosity. Sensitivity analysis helps predict how small changes in these parameters can lead to significant variations in fluid behavior.
Hypercomplex differentiation has been successfully used to calculate high-order derivatives of nonlinear problems [1]. In our approach, we apply Order-Truncated Imaginary (OTI) algebra for conducting sensitivity analysis on fluid simulations. This method enables high-order differentiation and is computed as a postprocessing phase, thus not interfering with the finite element simulation [2]. The process begins by determining the solution at each node for a specific time step, achievable through various simulation software. Following this, we compile the global tangent matrix. Subsequently, we establish a system of equations and calculate the imaginary components of the solution, which contain the derivatives with respect to design parameters. OTI algebra facilitates the assessment of sensitivities in fluid dynamics problems as a postprocessing activity, eliminating the need for additional computational resources in the finite element analysis. High-order derivatives of the fluid velocity were computed using the presented methodology. Results showed excellent agreement when compared to known analytical solutions.

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Modeling and simulation of advanced manufacturing processes for metals
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL AND EXPERIMENTAL ANALYSIS OF PEEL FAILURE PROGRESSION IN ADHESIVE JOINTS OF GFRP VIA T-PEEL TEST

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ABSTRACT

This paper focuses on numerically modeling peel failure in adhesively bonded fiberglass reinforced composite (FRP) joints, employing T-peel tests to investigate the influence of fiber orientation, adhesive thickness, and substrate thickness on peel strength. The applied methodology, utilizing the serial/parallel mixing theory as a constitutive law manager, is complemented by the integration of constitutive models capturing damage in both the adhesive and substrate. This cohesive approach enables a nuanced representation of the interaction between these materials, specifically modeling the substrate-adhesive interface.

To validate results, a design of experiments is carried out that examines the thickness of the adhesive, the number of substrate sheets and different fiber orientations. The validity of our approach is confirmed by obtaining accurate comparisons with experimental results.

The applied approach, which employs a numerical modeling based on serial-parallel mixing theory and constitutive damage models, results in a robust tool for adhesive bond design and optimization, as it accurately predicts peel failure propagation and also provides a deeper understanding of the failure mechanism by providing a stress distribution along the substrate-adhesive interface.

Lattice Boltzmann modelling and study of complex flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STOCHASTIC DESIGN OF MULTI-MATERIAL WELLBORE PLUG PLACEMENT PROCESSES

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ABSTRACT

Plugging orphaned and abandoned wells with a combination of bentonite clay gel and cement slurry has emerged as a cost-effective strategy for preventing the migration of unwanted fluids and ensuring zonal isolation. Despite the efficacy of this approach, challenges persist, such as the potential loss of the bentonite component of the plug and unexpected leakage. Prior work has shown the capability of the Lattice Boltzmann Method (LBM) to estimate the resulting plug positioning and other important factors when placing layered multi-material plugs comprised of bentonite clay gel and cement slurry (Garcia, et al. 2023). The current research builds upon this previous work by expanding the plug placement analysis, and ultimately design approach to incorporate the ubiquitous uncertainty that exists in plug placement processes, including variability in wellbore conditions (e.g., borehole diameter) and process parameters (e.g., pumping velocity). As previously, the LBM is used as the deterministic solver to simulate the effects of the rheological properties of cement slurry and bentonite clay gel, as well as wellbore condition in wellbore plugging operations, due to its capability to capture the complex fluid interactions inherent in multi-material systems. The LBM is then combined with a Monte Carlo approach that uses response surface modeling for computational efficiency to evaluate the effects of uncertainty in the system parameters on the plug placement process. In addition to the details of the analysis strategy, results will be presented examining the effects of the rheological properties of cement slurry and bentonite during realistic plug placement scenarios accounting for uncertainty. Moreover, this analysis will be used to explore the design elements of the plugging process (e.g., material properties, pumping velocity, etc.) that are needed to ensure reliable plug placement to achieve zonal isolation.

VIRTUAL ELEMENT APPROXIMATION OF EIGENVALUE PROBLEMS

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ABSTRACT

Virtual Element Methods (VEM) for the approximation of PDE eigenvalues problems has been adopted and analyzed by several authors, starting from standard elliptic problem, including hp VEM, nonconforming VEM, and mixed schemes, the Steklov eigenvalue problem, plate models, linear elasticity, to transmission problems.
An important feature of VEM, as compared to standard FEM, is that suitable stabilizing forms, depending on appropriate parameters, have to be introduced in order to guarantee consistency and stability of the approximation. Indeed, as it is well known, the matrices assembled for the discretization are computed by the use of suitable projection operators. This is due to the virtual nature of the basis functions corresponding to the degrees of freedom at the interior of the elements. The lack of knowledge of such basis functions is compensated by adding appropriately chosen stabilization terms. Typical theoretical results state that, for given choices of the stabilization parameters, the discrete solution converges to the continuous one with optimal order asymptotically in h or p. It is implicitly understood that the convergence behavior depends on the choice of the parameters.
Recently, it was observed [1,2] that in the case of eigenvalue problems, the presence of the stabilizing partameters may introduce artificially additional eigenmodes and we have to make sure that they will not pollute the portion of the spectrum we are interested in.
In [1] we presented a systematic study of the eigenvalue dependence on the parameters. If the discrete eigenvalue problem can be written in the form $Au = \lambda Mu$, with A and M depending linearly on the stabilizing parameters α and β, respectively, then the quick and easy recipe is to pick a sufficiently large α and a small (possibly zero) β.

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Advances in numerical methods for solution of PDEs
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CONSISTENT, ACCURATE UNSTEADY ADJOINTS FOR MESH AND MODEL ADAPTIVITY

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ABSTRACT

We present general, automated adjoint techniques and implementations for implicit unsteady solvers. Particular attention is paid to the correctness and consistency of the adjoint error estimate, which reveals a non-intuitive adjoint weighting for implicit-Euler timesteppers. The unsteady adjoint is used to drive mesh adaptivity between timesteps, while an adaptive time solver is used to adapt timesteps, providing a spatio-temporal adaptive numerical scheme. Numerical experiments illustrate the role of the adjoint solution in revealing and resolving non-local sources of error for both the space and time discretization.

SciML in the real world
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INFERENCE OF FOKKER-PLANCK EQUATIONS FOR THE DYNAMICS OF POPULATIONS

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ABSTRACT

The population dynamics of a wide range of systems from human agents to biological cells evolve in response to internal rules. One common approach to them is via Markov Decision Processes, which address these problems by considering agents that take actions following a probabilistic policy function to make transitions between states. Also included in this framework is the notion of a reward function that the agents maximize by choosing an optimal policy. Such a description can be arrived at by algorithms of inverse reinforcement learning, which, however depend on the specification of the transition probability function. While the transition function may be constructed empirically, it may miss important mechanistic information and not generalize well. This has led to interest in obtaining the transition function by first inferring a partial differential equation--typically one that has the form of an optimal transport problem--from the data. When applied to real data that is multi-modal, represents high-dimensional probability densities, and furthermore is sparse, the optimal transport form may be difficult to learn. Here, recent advances in learning complex, push-forward maps of distributions assume importance. They allow the identification of optimal transport forms underlying non-Gaussian distributions. Furthermore, with the Fokker-Planck equation, they also allow the inference of the potential and diffusivity in parametric form. This is of special interest in the setting of cell dynamics where the potential field can arise from chemokine gradients and diffusivity models the random migration of cells. We will discuss recent advances in the inference of high-dimensional Fokker-Planck equations for this class of problems.

EFFECTS OF DIFFERENT ARCHITECTURAL CHOICES FOR AUXETIC METAMATERIALS ON IMPACT MITIGATION

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ABSTRACT

For the mitigation of high-velocity impacts in military or space context, such as bullet and fragment impacts on personal protective equipment or space debris endangering satellites at orbital velocities, auxetic (negative Poisson's ratio) materials are claimed to offer distinct advantages. These materials provide enhanced indentation resistance, shear resistance, fracture toughness, and energy adsorption [1]. Auxetic materials are rare in nature and must be artificially designed. The process of designing materials with desired static properties is well understood in the linear regime. However, there has been little attention given to the behavior of architected materials under finite deformations at high deformation rates, which are expected during impact events. The resulting microstructural changes and how they affect the desired properties are not yet well understood.
A design and optimization process of these metamaterials, informed by their behavior in high-velocity impact, is necessary to enable the development of lightweight protective structures. Computational tools are needed to help engineers design these structures with the challenges of high-velocity impact scenarios in mind and to ensure a fast and reliable design process. For these tools a solid understanding of the material behavior under large deformations and high rates, including the highly dynamic and nonlinear effects in the heterogenous metamaterials, is crucial. A solid numerical representation of lattice structures is essential in achieving this understanding.
This research examines the effects of changes to the geometry due to large deformations at high strain rates in architected auxetic lattice materials. It presents the modelling of these lattice structures as an assembly of nonlinear beams in both static and dynamic conditions. We discuss the changes in the internal structure of different architectures and the subsequent response to localized high velocity impacts. To ensure a fair comparison, we first design various auxetic architectures with the same initial linear properties. We then illustrate the differences in the evolution of these properties under simple deformation modes and relate them to the observed variations in the impact mitigation performance of the studied architectures. We also illustrate the geometrical features of these architectures and their influence on the response. Finally, we demonstrate the performance of the nonlinear computational model through relevant numerical examples.

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LAGRANGE MULTIPLIER APPROACHES FOR THE FINITE ELEMENT APPROXIMATION OF INTERFACE PROBLEMS

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ABSTRACT

This talk is devoted to the finite element approximation of boundary value problems with interfaces. We shall consider a simple second order elliptic equation with discontinuous coefficients and present the most common approaches for its finite element discretization. One main feature of these methods consists in the construction of the mesh which can befitted or unfitted. In the first case the mesh is constructed such that the elements are not cut by the interface, so that the resulting approximation has optimal rate of convergence according to the regularity of the solution.
Unfitted meshes are independent of the position of the interface, leading possibly to non optimal rate of convergence of the approximation. In particular, we shall present methods based on the introduction of a Lagrange multiplier to enforce weakly the transmission conditions across the interface using unfitted meshes. These approaches can be efficiently extended to the finite element approximation of fluid-structure interaction systems.

Computational methods in environmental fluid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFICIENT NUMERICAL SCHEMES FOR DEPTH-INTEGRATED LANDSLIDE RUNOUT MODELS

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ABSTRACT

The development of landslide early-warning systems is of paramount importance for cities located in mountainous areas.
Landslide dynamic encompasses various velocity scales and mechanical behaviors, presenting challenges in numerical modeling. In this work, we focus on landslide runout phase. While the comparison of the horizontal propagation length scale of the landslide with
the vertical one suggests the use of depth-integrated models, the different behavior of various types of landslide, such as debris flows and mudflows, entails the need to define more detailed mathematical models.

Two numerical frameworks are proposed: one for homogeneous moving slides, such as mudflows, and the other for landslides with significant solid-liquid interactions. These schemes adopt adaptive mesh refinement and domain partitioning on hierarchical quadtree meshes, enhancing scalability and efficiency. These numerical schemes can be seen as modifications of the standard two-step Taylor-Galerkin (TG2) scheme on quadtree meshes. We propose modifications aimed at ensuring well-balancing property and overcoming the numerical stiffness coming from diffusion-reaction terms, while guaranteeing scaling performances proper of the TG2 scheme. To ensure the well-balancing property we resort on a novel implementation of the path-conservative strategy in TG2 scheme and employ either second-order operator splitting methods or implicit-explicit additive Runge-Kutta scheme to face numerical stiffness coming from the finite-element discretization of diffusion-reaction terms.

Numerical experiments demonstrate the effectiveness of the schemes in terms of time-step selection, parallel performance, accuracy, and ability to deal with real topographies.

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Machine learning for design tasks and inverse problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SOLVING DISTRIBUTIONALLY ROBUST SHAPE DESIGN PROBLEMS BY LEARNING SHAPE DERIVATIVES

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ABSTRACT

Recently, a robust design optimization framework based on distributionally robust optimization (DRO) was proposed in [1]. DRO aims to minimize the worst-case expected performance in a set of distributions that is informed by observed data with uncertainties. It allows a new perspective to the formulation of robust design optimization problems, which is classically based on the mean-variance (standard deviation) optimization formulation pioneered by Taguchi [2]. Notably, DRO allows data-driven and statistically principled ways to quantify the trade-offs between robustness and performance, which contrasting the classical robust design formulation that captures uncertainty only qualitatively.

This study focuses on the solution of distributionally robust shape design problems in which the function and gradient evaluations are expensive. To accelerate the solution of the min-max design problems, we present a computational framework that learns not only the forward solution of an engineering problem, but also the respective first-order information, in our case, the shape derivatives. We will present computational results on complex engineering design problems, where the data for the training are obtained using the open-source software SU2.

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Fluid-structure interaction in interface and moving boundary problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MULTISCALE IMMERSED BOUNDARY FRAMEWORK FOR ACOUSTIC STREAMING

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ABSTRACT

Key Words: Acoustic Streaming, Immersed Boundary, Multiscale Methods

The integration of acoustics and microfluidics (“microacoustofluidics”) has shown great promise for precise manipulation of fluids and particles at microscales. Microacoustofluidic systems typically entail propagation of high-frequency acoustic waves through viscous fluids. Owing to the dissipation of the acoustic wave in viscous fluids, the fluid response is characterized not only by a high-frequency response of the fluid, but also by a slow mean flow, referred to as acoustic streaming. This nonlinear interaction of acoustic waves with viscous fluids can be harnessed to realize acoustically propelled microswimmers that can offer precise, tunable motion at microscales [1]. However, while acoustic streaming flows have been extensively studied, the understanding of immersed moving objects within streaming flows remains a work in progress.

In this work, we present an immersed boundary formulation to model the motion of acoustically propelled microswimmers. We leverage an explicit time scale separation approach to split the problem into a periodic first-order problem that models the fluid’s high-frequency response, and a second-order time-averaged problem that describes the fluid’s mean response [2]. Notably, the second-order system is solved in terms of fluid’s mean Lagrangian velocity that significantly facilitates its coupling to the immersed object. The proposed formulation is numerically implemented within the open-source Immersed Boundary Adaptive Mesh Refinement (IBAMR) framework [3]. In addition to the details of the formulation and its implementation, we present numerical test cases to highlight the salient features and capabilities of our implementation.

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Transport phenomena in micro/nanofluids
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ENHANCED HYDRODYNAMIC DIFFUSION IN DENSE BINARY ACTIVE SUSPENSIONS

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ABSTRACT

Active suspensions are fluids loaded with microscale energy-injecting particles such as cells, bacteria or active colloids. Because they are intrinsically out-of-equilibrium, active suspensions can display a number of fascinating phenomena, including enhanced diffusion, "bacterial turbulence", and even a "superfluidic" rheology.

Here, we numerically study the effect of incorporating passive particles into a dense active suspension using the Fast Stokesian Dynamics method. Specifically, we focus on individually immotile active particles, whose collective dynamics arise from the activity-induced many-body hydrodynamic interactions. In the absence of Brownian motion, both active and passive particles fluctuate vigorously in space, displaying pronounced hydrodynamic diffusion. The rotational diffusivity of all particles decreases monotonically with the fraction of passive ones; however, surprisingly, the translational diffusivity is nonmonotonic and can be significantly enhanced. This suggests a hydrodynamic coupling of the translational and rotational dynamics, which we find can be attributed to local ordering of the active particles as a result of hydrodynamic interactions. Using a toy model, where passive particles are treated as defects in a lattice of aligned force dipoles, we reveal a simple mechanism by which spatial correlations and inactivity give rise to enhanced diffusion. Our results uncover an unexpected effect of passive particles on the dynamics of active suspensions, providing new possibilities to enhance mixing and modulate mass transport in active fluids.

Modeling and simulation of coupled processes in geological media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE THERMO-MECHANICAL INTERACTIONS OF FAULT FRICTION

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ABSTRACT

The frictional behaviour of rocks and fault surfaces is important to a wide range of geological processes such as earthquake nucleation and induced seismicity. The frictional properties of rocks depend on many parameters including velocity, stress, temperature, chemistry, and material properties. The frictional behaviour is complex – for example, some rocks have been shown to transition from velocity-strengthening to weakening then back to strengthening as the rock temperature is increased [1]. In-situ fault conditions combine all these properties simultaneously leading to multi-physics behaviour that cannot be adequately studied at the laboratory scale.

While fault movement is a multi-physics phenomenon combining lubrication, chemistry, and deformation, here we focus primarily on the thermo-mechanical behaviour of fault movement. There is a strong two-way coupling behaviour as fault movement under large in-situ stresses induces significant flash heating of the fault surface [2]. The heating causes thermo-elastic expansion near the fault surface, which increases the contact stress, but the heating also softens and potentially melts the rock mass. The heating of the rock mass changes the stress state and frictional properties, which in turn changes the rate at which heat is generated.

In this study, we build a coupled numerical model to examine the in-situ thermo-mechanical behaviour of fault friction. We discuss the development of the numerical model and coupling methods, as well as the associated numerical challenges including contact, steep temperature gradients, large model scales, and convergence. We consider traditional friction models including the Coulomb and rate-and-state friction laws and compare them to more modern constitutive laws. We examine the thermo-mechanical effects and compare them to laboratory observations to determine which observed frictional effects can be attributed to coupled thermo-mechanical behaviours and which must be attributed to other factors. Last, we discuss the implications of geochemistry and lubrication on the coupled in-situ fault friction behaviour.

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Mathematics and algorithms for predictive digital twins (DT)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LEARNING PHYSICS-BASED REDUCED-ORDER MODELS FROM DATA USING NONLINEAR MANIFOLDS

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ABSTRACT

The rapidly increasing demand for computer simulations of complex physical, chemical, and other processes places a significant burden on the shoulders of computational scientists and engineers. Despite the remarkable rise of available computer resources and computing technologies, the need for model order reduction to cope with these problems is an ever-present reality. Reduced-order models are imperative in making computationally tractable outer-loop applications that require simulating systems for many scenarios with different parameters and under varying inputs. They require that one numerically solves the differential equations describing the physical system of interest in low-dimensional reduced spaces, in contrast to the original full-order models. However, traditional model reduction techniques often fail to identify a low-dimensional linear subspace for approximating the solution to many physics-based simulations.

In this talk I will present a novel method for learning projection-based reduced-order models of physics-based dynamical systems using nonlinear manifolds. First, we learn the manifold by identifying nonlinear structure in the data through a general representation learning problem. The proposed approach is driven by embeddings of low-order polynomial form. The algebraic structure of the system that governs the problem of interest in the reduced space is revealed by means of a projection onto the nonlinear manifold. The matrix operators of the reduced-order model are then approximated, in a least-squares sense, using data-driven operator inference. Numerical experiments on a number of nonlinear problems demonstrate the generalizability of the methodology and the increase in accuracy that can be obtained over standard POD-based methods.

Data-driven methods for modeling complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN FUNCTIONAL NETWORKS FOR COMPLEX RESPONSE ANALYSIS

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ABSTRACT

Network methods are a growing field of data-based approaches to the modeling and analysis of complex dynamical systems. These complex networks provide a complementary perspective to classical physics-based or neural network-based approaches, where the resulting model is often a black box. In this alternative approach to data-based modeling, networks formed by nodes connected via edges represent uni- or multivariate data sets. The complex network is obtained from measurement data using physics-based measures, such as recurrence properties. Network methods are popular in many disciplines, such as biology, climate research, and medicine. Examples of practical applications include determining coupling properties between different system components, tracking transient phenomena such as regime changes, and anomaly detection.

In this work, we use a recurrence-based network algorithm to generate a functional network from a synthetic data set of displacements of different model components. The underlying dynamical system is a classical model for a bladed disc, as in a wind turbine. The model consists of cyclically coupled nonlinear oscillators, which are known to exhibit complex dynamical behavior. In the functional network, each node represents a physical component of the model, and each edge represents a functional relationship between two elements. More precisely, the network nodes are connected based on a recurrence-based functional dependency obtained from the displacement time series, instead of their geometrical proximity or physical coupling.

The functional network reveals important information on the underlying dynamical system, such as the dimension of the dynamics in phase space. The network can also follow the propagation of an external disturbance through the system and track dynamical transitions stemming from changes in system parameters. These findings may provide a basis for a more efficient system analysis through better sensor placement based on determining relevant measurement locations. It can also help develop effective countermeasures against unwanted disturbances or vibrations in specific parts of the machine by exploiting the path the disturbance takes through the system. Additionally, early warning methods for critical transitions can be developed based on the functional network methods.

Uncertainty quantification and reliability analysis in engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NEW PARADIGM FOR ENGINEERING SIMULATIONS UNDER UNCERTAINTIES: TIME-SEPARATED STOCHASTIC MECHANICS

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ABSTRACT

The widespread use of uncertainty quantification in engineering simulations is severely hindered by the lack of fast and accurate methods that can handle inelastic material behavior and local material fluctuations. Many existing methods in the framework of stochastic finite element methods can only be employed for linear elastic or simplified polynomial material models.

In contrast, the time-separated stochastic mechanics was directly developed for the fast and accurate uncertainty quantification of structures with inelastic material response.
The method is based on a separation of both of the system equations, i.e. the balance of linear momentum and the evolution equation for the internal variable(s), into stochastic but time-independent and deterministic time-dependent terms. This allows to approximate the stochastic behavior with a low number of fast deterministic FEM simulations and several fast matrix calculations. In comparison to classical Monte Carlo simulations a significant speed-up combined with a high accuracy can be be observed.

In this talk, we present the application of this promising new approach for the inclusion of stochasticity for a variety of different problems as viscoplastic materials, damage simulations and phase transformations.

LINEAR AND NON-LINEAR DIMENSION REDUCTION STRATEGIES FOR MULTI-FIDELITY SAMPLING UNCERTAINTY QUANTIFICATION: COMPLEXITY VERSUS PRECISION

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ABSTRACT

Multi-fidelity sampling approaches are emerging as effective techniques for the evaluation of statistics of high-fidelity models, whenever the number of available evaluations is limited. In principle, these approaches work by leveraging the statistical correlation among quantities of interest generated by several data sources, and lead to a reduced estimator variance by combining the limited number of high-fidelity evaluations with a large number of low-fidelity model outputs (e.g., [1,2]). Unfortunately, for realistic applications in science and engineering, the correlation between low- and high-fidelity model outputs can be limited as a result of a different parameterization. For instance, the low-fidelity model can be formulated in terms of a simplified constitutive or closure model (e.g., Reynolds-Averaged Navier Stokes turbulence model) defined using a different number of parameters than the high-fidelity model (e.g., Large Eddy Simulation).

In recent studies [3,4], we have demonstrated that a shared input parameterization can be created by relying on low-dimensional manifolds. This shared parameterization is often capable of significantly increasing the correlation between models, thus enhancing the overall performance of multi-fidelity sampling strategies.

In this talk, we will consider both linear (Adaptive Basis, AB) and nonlinear (Auto-Encoders, AE) dimensionality reduction strategies to understand the computational trade-off between the complexity of identifying a shared manifold and the resulting correlation increase. We will also quantify the overall performance of the multi-fidelity estimators associated with these approaches. Finally, we will consider extensions of the estimators introduced in [3,4] that include the use of low-dimensional manifolds with dimensions greater than one, and the use of multiple low-fidelity models. We will illustrate the computational challenges associated with these extensions, and consider multiple test cases to compare and contrast strategies based on AB and AE.

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Towards predictive digital twins: Innovative algorithms for physics-, data-assisted and hybrid modeling
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INTELLIGENT DECISION SUPPORT SYSTEM FOR RAIL SANDING SYSTEM

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ABSTRACT

Low rail adhesion has a significant safety and financial impact on the railway industry and society (estimated at £350m/year in the UK). Currently, this phenomenon is managed by depositing dry sand through an onboard system that the operator subjectively controls while, inevitably, neglecting several efficiency factors. However, both contamination and sanding cause surface damage, wear, and fatigue of railway tracks. Additionally, if not adequately controlled, an excessive amount of sand can interface with the ability of track circuits to detect a train, called wheel-rail isolation, causing safety issues. Accordingly, a prominent need was identified by the research and industry communities for analysing the several parameters that affect the rail sanding systems' efficiency and determining optimal decisions regarding the application of these systems.

Whilst sanding parameters such as the location of the nozzle, frequency of application, and angle of attack have been extensively studied, the lack of understanding of the physical and chemical processes at rail-wheel interfaces has been acknowledged by industry experts to be of key importance and fundamental to overcoming the challenges. Additionally, accounting for the inherent subjectivity associated with the human decision-making process is essential for communicating the results of such analysis with train operators more effectively.

In this project, we have developed an intelligent and intuitive framework to support train operators in making rail sanding decisions in real time. Our framework, named INSURERS (INtelligent deciSion sUppoRt systEm for Rail Sanding), utilises a high-fidelity digital twin of rail sanding systems and combines it with advanced machine learning and granular computing techniques to deliver an intelligent and intuitive framework train operation in low adhesion conditions.

Our first contribution is utilising deep learning to replicate our high-fidelity discrete element modelling of rail sanding systems [1], which significantly reduces the simulation computational cost; hence, we realised the use of high-fidelity digital twin frameworks in real-time applications. Our second contribution is using granular computing to replicate human's subjective decision-making process. Human decisions are often made based on subjective assessment of their surrounding environment (e.g., "low" adhesion, "very low" temperature). Consequently, an intuitive decision-support system needs to replicate such subjective decision-making procedures [2]. Our future contributions will include the quantification of human factors and field measurement in the proposed framework.

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FLEXIBLE MACRO-MICRO COUPLING FOR SPATIAL SIMULATION OF THE LIVER

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ABSTRACT

Liver disease is one of the leading causes of death in the developed world. Because irreversible liver damage and end-stage liver disease may require high-risk surgery such as liver resection or transplantation, simulation-based risk assessment has enormous potential for clinical application [1]. For example, personalized drug dosing and pharmacokinetics can be simulated prior to actual treatment. Here, we present a flexible macro-micro coupling based on the interplay between the tissue and the cellular scale using FEBio, libRoadRunner and preCICE [2]. The deformation, flow and transport processes at the macro scale are represented by a system of coupled partial differential equations (PDEs) within the Theory of Porous Media (TPM). The described advection-diffusion system is extended by reaction terms that model cellular functions such as metabolism of the hepatocytes that form the tissue matrix. Each hepatocyte can be modeled as an individual microsimulation using ordinary differential equations (ODEs). Reproducible and efficient data communication between the domain-specific solvers FEBio (PDE) and libRoadRunner (ODE) can be achieved using the coupling library preCICE. The micro simulations are adaptively controlled by the MicroManager [3], a software tool of the preCICE ecosystem. libRoadRunner uses the Standard Biology Markup Language (SBML) as input format and provides a flexible model exchange to couple different systems on the micro scale. On the macro scale, generic software layers are used to maintain the flexibility of FEBio. We demonstrate the system using the example of the SPT model, which describes the conversion of a substrate (S) into a product (P) with the formation of a toxic by-product (T) as a showcase.

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APPLICATION OF GPU PROCESSING TO THE ELASTIC-PLASTIC IMPACT CODE (EPIC)

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ABSTRACT

Graphics Processing Units (GPUs), specialized chips designed to help computers render large numbers of 3D geometries, have been increasing in computational power over the years. Because they are designed to do similar computations for millions of objects, the GPU has been optimized for the single-instruction-multiple-data (SIMD) computing model. As GPUs have become more powerful, they have been applied to many different computational mechanics problems. For some problems, like using the spectral method on crystal plasticity, the vast majority of the problem can be done on the GPU, leading to remarkable speed-ups compared to running on a general-purpose Central Processing Unit (CPU).

For Lagrangian Finite-Element problems, GPUs can be helpful for certain algorithms in the code, such as the strain/stress computations in the finite elements and meshless particles, but they will not be efficient for every algorithm. The Elastic-Plastic Impact Code (EPIC) is both a research and production Lagrangian Finite-Element code that has been primarily funded and used by various branches of the Department of Defense (DoD). EPIC has long used the Message-Passing Interface (MPI) for parallelism, and has more recently added OpenMP compiler directives (which also use the SIMD computing model). OpenMP can be used in conjunction with MPI to increase EPIC's scalability. Using GPUs via the OpenACC programming interface instead of OpenMP for the thread-based parallelism will open up further possible speedups of the stress/strain computations for both elements and particles, as well as the contact algorithm.

This presentation will show the relative speeds of doing the element, particle, and contact computations on CPUs and GPUs on various architectures.

Geometric mechanics formulations and structure-preserving discretizations for continuum mechanics and kinetic models
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MIMETIC SPECTRAL ELEMENT DISCRETIZATION OF CONTINUUM MECHANICS

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ABSTRACT

In mimetic discretization methods we distinguish between conservation laws, definitions and constitutive laws. Since conservation laws and definitions are topological, we demand that these relations are discretized without any reference to discretization parameters such as the element size, time step or polynomial order used in the method. The metric-dependent part in which these numerical parameters do appear, stems from the constitutive relations, which, in turn, follow from the energy relations.
In this talk all physical variables will be interpreted as (co)vector-valued differential forms and duality will be employed to design a discretization which meets the above requirements.
As an example, the mimetic spectral element method is applied to an elasticity problem, [1,2] for which exact conservation will be demonstrated.

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THE INTERNODES METHOD FOR THE SOLUTION OF PDES IN MULTIDOMAIN SETTINGS FEATURING NON-CONFORMING INTERFACES

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ABSTRACT

The Internodes method is an interpolation-based approach for dealing with the solution of PDEs in domains partitioned into non-overlapping subregions featuring non-conforming interfaces. The non-conformity could be of geometric type (non-watertight interfaces) and/or discretization type (when the mesh sizes and/or the local polynomial degrees inside the subdomains differ). The discretization inside each subdomain can be achieved by a Galerkin-based method, e.g., Finite Elements, Spectral Elements, or Isogeometric Analysis.

The method was introduced in [1] and its convergence was analyzed in [2] for hp−fem. In particular, when the mesh sizes in the two adjacent subdomains decrease uniformly, then the method achieves optimal convergence in the broken-energy norm with respect to the maximum mesh size, exactly as the well-celebrated Mortar method does. Moreover, it has been proved that Internodes is conservative, that is it preserves some quantities (typical of the continuous solution of the specific PDE) at the interface of the decomposition. For example, in the case of linear elasticity problems, it preserves the balance of the forces and the null total work at the interface. The Internodes method has been applied with success to multiphysics problems, contact problems, and, recently, in the context of Reduced Basis Methods [3].

In this talk, I will present the Internodes method and its applications in different contexts, as a result of the collaboration with many co-authors: Pasquale Africa, Guillaume Anciaux, Michele Bucelli, Agnese Dall'Olio, Simone Deparis, Davide Forti, Andrea Manzoni, Federico Marini, Alfio Quarteroni, Yannis Voet, Filippo Zacchei, Elena Zappon.

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Advanced numerical techniques for fluid flow in porous media
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STABILITY OF NANOSCALE GAS BUBBLE TRAPPED BY A SURFACE DEFECT: A MOLECULAR DYNAMICS STUDY

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ABSTRACT

Surface defects are known to be able to trap and stabilize nanobubbles, which can impact applications in industry, such as improving the separation process [1] and reducing drag force [2]. The stability of nanobubbles is highly depend on thermodynamic conditions and fluid properties as well as surface characteristics such as wettability and defect shape. Although a few mechanisms, such as oversaturation and contact line pinning, have been proposed in the literature, there are controversial opinions which are rooted in the limited resolution of experimental approaches [3]. In this work, molecular dynamics simulations are performed to investigate how the stability of a nanobubble trapped in a surface defect (cavity) is affected by the shape of the cavity, surface wettability, and the gas type. For this purpose, the investigation considers two cavities with the same opening width and depth (one V-shaped and the other square-shaped), two types of silica-based surfaces with different levels of wettability (hydroxylated and methylated, the former having greater water wettability), and two types of gas (carbon dioxide and nitrogen). The results show that regardless of the cavity shape, the gas molecules have a higher probability to position close to the corners of the defects. The square-shaped cavity exhibits better capability in adsorbing and stabilizing the gas molecules. Both nitrogen and carbon dioxide are able to form hydrogen bonds with the hydroxylated silica, enhancing their stability near the surface. However, nitrogen shows stronger hydrogen bonding. Together, the highest nanobubble stability is observed for the nitrogen trapped in the square-shaped cavity of the hydroxylated silica. Results revealed from molecular simulations can be used to design surface features that are better at trapping and stabilizing nanoscale gas bubbles without changing thermodynamic conditions or fluid properties.

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16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics

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NEW PARADIGMS IN DATA ASSIMILATION

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ABSTRACT

Partial differential equation provide a map from initial/boundary conditions and parameters to field variables that vary at each point of space and time. This level of completeness, while suitable for understanding the behavior of physical processes, is often too detailed for the purpose of data-based inference. This is because, often, operational and experimental measurements pertain to patterns that form coherent structures that are not, themselves, constrained by the same physical laws as the field variables. This situation is increasingly common with modern sensing capabilities that are matched with flagship simulation resources.

In this talk I will describe a new paradigm for data assimilation that is adapted to this reality. The new methodology maintains a firm grounding in probabilistic concepts while permitting statistical conditioning on arbitrary observables and inferences about equally arbitrary quantities of interest. I will show examples from a variety of applications that include materials science and reactive flows.

Mathematics and algorithms for predictive digital twins (DT)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DERIVATIVE-INFORMED NEURAL OPERATORS FOR PREDICTIVE DIGITAL TWINS

Omar Ghattas[1], Lianghao Cao[2], Peng Chen[3], Dingcheng Luo[1], Thomas O'Leary-Roseberry[1] and Umberto Villa[1]*

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ABSTRACT

A digital twin is a computational model of a physical system that continually updates its knowledge of the system by assimilating observational data, and in turn informs decisions and controls the system to achieve a desired goal, over a continually evolving time horizon. When the model takes the form of a system of PDEs, and when the data assimilation and optimal control problems must be solved under uncertainty, the computations underlying digital twins quickly become prohibitive. Efficient surrogates of the maps from parameters and decision variables to quantities of interest, which involve solution of the forward PDEs, is key to making digital twins tractable. Unfortunately, constructing such surrogates presents significant challenges when the parameter/decision dimension is high and the forward model is expensive, which limits the amount of available data.

Deep neural networks (DNNs) have emerged as leading contenders for overcoming the challenges of constructing infinite dimensional surrogate models. These have become known as neural operators. We show that black box application of DNNs for problems with infinite dimensional parameter fields leads to poor results when training data are limited due to the expense of the model. Instead, by constructing a network architecture that captures the geometry of the map---in particular its smoothness, anisotropy, intrinsic low-dimensionality, and input-output derivatives---one can construct a dimension-independent reduced basis neural operator that is accurate and optimization-aware using limited training data. We employ this reduced basis neural operator to make tractable the the solution of PDE-constrained Bayesian inverse problems and optimal control under uncertainty. Applications are shown to problems governed by wave propagation, hyperelasticity, and viscous flows.

Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOWARDS REAL TIME BAYESIAN INVERSION AND PREDICTION OF MEGATHRUST TSUNAMIS

Stefan Henneking[1], Sreeram Venkat[1], Milinda Fernando[1] and Omar Ghattas[1]*

[1]The University of Texas at Austin

ABSTRACT

Tsunamis generated from megathrust earthquakes are capable of massive destruction. Efforts are proceeding to instrument subduction zones with seafloor acoustic pressure sensors to provide early warning for tsunamis. Our goal is to employ this pressure data, along with the coupled acoustic–gravity wave equations, to infer the spatiotemporal seafloor motion in a real time early warning system. The solution of this inverse problem then provides the boundary forcing to forward propagate the tsunamis toward populated areas along coastlines. Solution of the forward problem alone—the acoustic-gravity wave equations in a 3D compressible ocean—entails severe computational costs stemming from the need to resolve ocean acoustic waves with wavelength of order 150 m in a subduction zone of length ~1000 km and width ~200 km. This can require O(minutes) on a large GPU cluster. The inverse problem formally requires thousands of forward wave propagations; thus our goal appears to be intractable. We propose a novel approach to enable the accurate solution of this pair of inverse and prediction problems in real time, i.e., in a few seconds. The key is to exploit the structure of the parameter-to-observable map, namely that it is a shift-invariant operator, and its block Toeplitz structure permits fast FFT diagonalization. We discuss the Bayesian formulation, consistent discretization, and fast GPU solution. Application to inference of earthquake-induced tsunamis on the Cascadia subduction zone will be presented.

Mechanobiology of cells, vesicles and biomembranes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MESOSCOPIC SIMULATIONS OF PROTEIN-INDUCED MORPHOLOGICAL CHANGES IN ENDOPLASMIC RETICULUM

Emad Ghazizadeh[*1] and Wylie Stroberg*[1]

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ABSTRACT

The endoplasmic reticulum (ER) represents a highly dynamic intracellular network, characterized by a complex arrangement of membrane tubules and sheet-like cisternae. This complex morphology is perpetually in flux, responding to environmental cues. Key to this adaptability are various proteins within the ER membrane, orchestrating its structure in response to internal and external signals. Among these proteins, Climp-63 plays a central role in shaping sheet-like membrane structures within the ER. Climp-63 achieves this by forming dimeric struts across the ER lumen, promoting the development of expansive cisternae. Within the ER lumen, the accumulation of unfolded proteins leads to increased pressure and subsequent expansion of the ER lumen. In a counterbalancing mechanism, Climp-63 dimers bind across the lumen, mitigating the expansion induced by elevated unfolded proteins. This equilibrium of ER membrane shape is contingent upon the dynamic interplay between Climp-63 concentration and the unfolded protein loads within the ER lumen, aspects that are not fully understood. This study aims to show mesh-free simulation of ER membrane under influence of protein-driven remodelling membrane and the unfolded protein loads using Mesoscopic Membrane-Protein (MesM-P) method providing experimental length and time scale which is unapproachable for all-atom and coarse-grained molecular dynamic method. The findings provide crucial insights into the adaptive nature of the ER, shedding light on its ability to swiftly respond to changing cellular conditions such as tubulation, protein oligomerization. Understanding these regulatory processes may have implications for unraveling broader cellular dynamics and may offer potential avenues for therapeutic interventions such as diabetes, cancer and aging in conditions influenced by ER dysfunction.

Physical models and reduced order models augmentation with data for physics-informed machine learning in real-world applications
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PERMAFROST AUGMENTED SIMULATION AND FORECAST USING SPECTRAL NEURAL NETWORKS

Chady Ghnatios[*1], Thibault Xavier[23], Laurent Orgogozo[23] and Francisco Chinesta[1]*

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[3]*Laboratoire Géosciences Environnement - CNRS*

ABSTRACT

Global warming is impacting several crucial Earth systems, with the permafrost being among the affected components. To assess and predict the consequences of global warming, a numerical cryohydrogeological study on water and energy transfer in a forested, continuous permafrost site is conducted using the open-source fluid dynamics engine, OpenFOAM, with a parallel high-performance computing solver for the numerical simulation of permafrost dynamics. The numerical results reasonably replicate the measured soil temperature profiles and the dynamics of infiltrated waters observed in previous biogeochemical studies of the site of interest. However, these simulations can be enhanced by assimilating experimental measurements into the model through the development of a hybrid modeling approach. This approach aims to improve the physical simulation by incorporating data while maintaining the stability and the predictive capability of the dynamic model.

This work proposes a hybrid modeling process involving a spectral decomposition of the physical solution, combined with a deep neural network, to predict the augmented solution and correct the simulation. The final hybrid solution demonstrates a significant improvement in simulation accuracy when tested against future measurements, which were not part of the training set. Leveraging the resulting hybrid model, predictions are made regarding permafrost behavior in the coming years based on the currently accepted global warming scenarios.

QUANTIFYING UNCERTAINTY AND TUNING HYPERPARAMETERS OF THE UNSCENTED KALMAN FILTER USING A PHYSICS-AWARE LOSS FUNCTION FOR JOINT STATE AND PARAMETER IDENTIFICATION OF DYNAMICAL SYSTEMS

Esmaeil Ghorbani[1], Quentin Dollon[2] and Frederick Gosselin[1]*

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[2]*Hydro-Quebec Research Institutes (IREQ)*

ABSTRACT

In this study, employing terminology akin to Physics informed neural networks (PINNs), we introduce a versatile physics-aware loss function designed for tuning the hyperparameters of the unscented Kalman filter (UKF). Selecting appropriate hyperparameters is vital for the performance of all Kalman filtering algorithms, a process that can be both time-consuming and challenging in various contexts. Our primary objective is to use the UKF to estimate the desired states and parameters of the underlying system based on a predefined parametric model. This is part of a larger project aiming to develop a data-driven digital twin for a hydro turbine. The innovative idea involves adjusting the hyperparameters in an external optimization loop, using a nonlinear mesh adaptive direct search algorithm (NOMAD) combined with a physics-aware loss function. A key benefit of this novel loss function is that it does not incorporate sensor data into the physics-aware loss function. Instead, it solely relies on estimated states and parameters to minimize the loss function and optimize the hyperparameters. Additional advantages include: 1) The UKF's ability to filter sensor data noise during the estimation process prevents fluctuations or overfitting in the tuning of hyperparameters; 2) The Physics-aware loss aids in quantifying the modelling and measurement uncertainty of the system, considering its underlying physics; 3) Since the loss function is uncorrelated to sensor data, the algorithm could function as a virtual sensor for systems with sparse sensor data; 4) The algorithm facilitates the identification of Multiphysics systems, especially when there's no direct measurement for specific physics aspects. For instance, it can identify the influence of an unobserved fluid state in fluid-solid interaction problems. We have selected various case studies to assess the performance of the loss function under extreme scenarios. These include systems with time-varying parameters, systems with large number of unknowns and sparse measurements, chaotic systems (like the Lorenz system), highly nonlinear systems (Bouc-wen model), and the wake oscillator problem in fluid-structure interactions. These extreme case studies are chosen in a way to demonstrate that our proposed loss function achieves better accuracy compared to traditional data-driven loss functions. We also compare the performance of the data-driven loss function with our new loss function and the results are presented.

Mechanobiology of cells, vesicles and biomembranes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

OPTIMIZATION BASED SYNTHESIS WITH DIRECTED CELL MIGRATION

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ABSTRACT

Collective behavior of biological agents such as herds of organisms and cells is a fundamental feature in the systems biology and in the emergence of new phenomena in the biological environment. Collective cell migration under a physical or chemical cue is an example of this fundamental phenomenon where individual cell migration is driven by the collective behavior of the neighboring cells and vice versa. The goal of this research is to discover the mathematical rules of collective cell migration using experimental data and testing the predictive nature of the models in independent experimental data. Such insight is made possible in this work with the hybrid use of dynamic mode decomposition (DMD) and optimal control theory. Both single and multi-cellular systems are simulated, including obstacle courses, using this framework. The results of this work show how cells collectively behave during their migration and also, opens the possibility of designing robotic cells for possible therapeutic purpose where the cell trajectory can be controlled.

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Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CRYSTAL PLASTICITY PHASE FIELD MODEL WITH CRACK TIP ENHANCEMENT BY CONCURRENT ATOMISTIC-CONTINUUM MODEL

Somnath Ghosh[1] and Kishore Nair*[1]

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ABSTRACT

Crack propagation in polycrystalline metallic alloys is a complex multiscale process due to the interactions between cracks and dislocations. Dislocations nucleating from a crack tip contribute to the plasticity evolution in the vicinity of the crack, as well as to the crack propagation process. This paper systematically develops a method for enhancing the defect energy, accounting for crack-tip nucleated dislocations in the Helmholtz free energy density functional associated with the phase-field formulation of crack evolution in a coupled crystal plasticity finite element phase field (CPFE-PF) model. A concurrent crystal plasticity FE - molecular dynamics (CPFE-MD) model is developed to provide a basis and reference for this development. The CPFEM-MD model contains a crack in the MD domain. Dislocations emitted from the crack tip in the atomic domain are identified, transformed into dislocation densities across the interface into the continuum domain and subsequently propagated. The crack tip nucleated dislocation densities are subsequently used in the defect energy augmentation by modifying the accumulated slip to account for their contribution. A special method of identifying crack tips from the crack phase-field is proposed. The resulting CPFE-PF model thus captures the atomic scale mechanisms and shows a noteworthy deviation in the crack path and evolution of state variables near the crack tip in comparison with predictions without these contributions. State variables such as the effective plastic strain due to nucleated dislocations in the CPFEM-PF are validated by comparing them with predictions by the CPFE-MD model. A systematic study of the deformation mechanisms of Ti-6Al in the presence of a crack is conducted. The concurrent CPFE-MD model is used to create a database of the dislocation density and other state variables in the vicinity of the crack. A novel Bayesian inference methodology operates on this database to identify critical state variables that affect the crack tip nucleated dislocation densities. A genetic programming-based symbolic regression (GPSR) method is implemented to derive the functional form of the dislocation density evolution in terms of the critical state variables. Using the modified defect energy formulation, the evolution of crack and other state variables is compared. A significant deviation of the crack path and rate of propagation is observed. In conclusion, the overall framework and the derived functional form can be incorporated into any continuum crack model to account for the atomistic crack tip dislocation nucleation mechanism, independent of the microstructure and loading conditions.

16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics

July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN BAYESIAN MODEL-BASED PREDICTION OF FATIGUE CRACK NUCLEATION IN NI-BASED SUPERALLOYS

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ABSTRACT

This paper develops a probabilistic predictive model for crack nucleation in the Ni-based superalloy Ren\'e 88DT under fatigue loading. In this process, it fuses several statistical, data-driven methods operating on micromechanical and experimental data, as well as important mechanistic observations. The model systematically reduces a large set of experimentally obtained microstructural data and corresponding crystal plasticity-based micromechanical simulation results to a three-dimensional posterior probability density function (PDF) for crack nucleation. The framework identifies the three most important crack-delineating state variables in the microstructural material volume, viz. (1) the von Mises stress, (2) the maximum plastic slip rate, and (3) the plastic defect energy. This selection process is performed in a automated, data-driven manner without external intervention. It follows a statistically unbiased approach that makes an informed decision, while accounting for numerous experimental microstructures and mechanical simulations. The entire procedure, ranging from processing of experimental EBSD and SEM data, multiscale simulations for creating a database, to the development of the probabilistic crack nucleation model is implemented through an automated computational pipeline. Four serial, connected modules comprised this pipeline, viz.

- Collection of local microstructural data after fatigue loading and the cleaning and processing of EBSD data;
- Development of a concurrent multiscale model with the embedded image-based 3D microstructure in a self-consistent homogenized material;
- Multiscale simulations with different experimental microstructures to create a database of relevant micromechanical state variables;
- Formulation of a Bayesian crack nucleation model that identifies crack nucleation sites from the database of local state variable fields.

A simplified crack nucleation indicator is formulated to integrate the parallel slip concepts into a single scalar model.

Advances in material model calibration for computational solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

OPTIMIZATION OF THE SPECIMEN GEOMETRY FOR ONE-SHOT DISCOVERY OF MATERIAL MODELS

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ABSTRACT

We recently proposed an approach for Efficient Unsupervised Constitutive Law Identification and Discovery (EUCLID), which exploits machine learning tools such as sparse regression [1], Bayesian learning [2], or neural networks [3] to automatically discover material laws independent of stress data, but solely based on full-field displacement and global force data obtained from mechanical testing. The displacement field can be measured on the surface of a target specimen via digital image correlation (DIC).

An important feature of the approach is that, in principle, the discovery of the material law can be performed in a one-shot fashion, i.e., using only one experiment. However, this capability heavily relies upon the richness of the measured displacement data, i.e., their ability to probe the stress-strain space (where the stresses depend on the constitutive law being sought) to an extent sufficient for an accurate and robust discovery process. The richness of the displacement data and the robustness of the discovery process are in turn governed by the specimen geometry.

In the present study, we aim to optimally design the geometry of the target specimen via density-based topology optimisation approach. In this fashion, we perform automatic specimen design by maximising the robustness of the solution, i.e., the identified material parameters, given noisy displacement measurements from DIC. In this contribution, we shed light on the objective function, the topology optimisation framework, and a range of optimised topologies for orthotropic elasticity.

Keywords: Optimised specimen geometry; topology optimisation; discovery of material models; one-shot discovery.

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Immersed-boundary variational methods: Theory, data structures, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

UNFITTED HIGH-ORDER HYBRIDISABLE DISCONTINUOUS GALERKIN METHOD WITH EXACT NURBS GEOMETRIES APPLIED TO MICROFLUIDICS SYSTEMS

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ABSTRACT

The simulation of multi-fluid systems entails a series of numerical challenges related to the complex flow features that may arise from the interaction of different materials. Although high-order methods have demonstrated superior accuracy with respect to low-order methods, the difficulties to automatically generate high-order, curved meshes still limit their applicability in realistic scenarios. In this context, immersed boundary methods provide competitive solutions to handle complex geometries. In this talk, an unfitted, high-order hybridisable discontinuous Galerkin (HDG) method for two-fluid incompressible Stokes flows is introduced [1]. Boundaries and interfaces are described using NURBS curves embedded in a fixed Cartesian grid. The proposed immersed HDG method is suitable to exactly treat the geometry of the boundaries and the interfaces, circumventing the technical challenges of generating a high-order, curved mesh fitting the NURBS. Accuracy and consistency of the method are obtained by combining (i) the NURBS-enhanced finite element method (NEFEM) to perform numerical integration along immersed NURBS and in elements cut by NURBS curves [2]; (ii) a Nitsche's formulation to impose Dirichlet conditions on embedded surfaces; (iii) an automatic degree-adaptive procedure relying on the superconvergence property of the HDG postprocessed solution. Exploiting non-conforming meshes, exact NURBS geometry and high-order approximations, the method provides high-fidelity results on coarse meshes, independent of the geometric features of the domain, and maintains unknowns only on the mesh skeleton as in standard HDG [3], without introducing any additional degree of freedom on non-matching boundaries/interfaces. Numerical examples demonstrating the accuracy and robustness of the method will be presented, even in the presence of badly cut cells or faces, showcasing the suitability of the discussed approach to simulate microfluidics systems described using CAD geometries.

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Contact and interface mechanics: Modeling and computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HYPER-DIMENSIONAL GAP FINITE ELEMENTS FOR THE ENFORCEMENT OF INTERFACIAL CONSTRAINTS

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ABSTRACT

In the classical theory of two-body contact, a single shared contact interface is considered between two continuum bodies, and is further discretized as such in the finite element setting. In general, however, the finite element mesh topology of two contacting bodies will be non-conforming at this shared interface, requiring the definition of a preferred or intermediate surface over which integral constraints may be evaluated. The specification of this interface is deemed to be somewhat arbitrary, but in practice the numerical solution of contact problems may exhibit sensitivity to the particular choice of intermediate surface. A further complication concerns the need to establish projective mappings between the discretized finite element surfaces and the chosen intermediate surface, particularly for the sake of evaluating the contact gap function between pairs of points on each of the two bodies.

As an alternative to the strategy previously described, a new methodology for the enforcement of contact constraints in the context of finite element analyses is proposed. The method entails an alternative representation of contact surface integrals by equivalently integrating over the interstitial – albeit degenerate gap volume between two contacting bodies. An auxiliary indicator field is defined on each body, and is used to represent the degenerate interstitial volume as a non-degenerate hyper-dimensional gap volume. Over this domain, the gradient of the continuously interpolated displacement field with respect to the indicator field yields the oriented displacement gap, which may be used in the formulation of contact inequality constraints. Discretization of the hyper-dimensional gap volume into conforming finite elements is explored, and is observed to offer several advantages over existing contact discretization methods: the proposed method does not require the computation of geometric intersections or projections; it exploits conventional Gaussian quadrature schemes to integrate the hyper-dimensional gap integrals with a sufficient degree of accuracy; and may be naturally and efficiently extended to represent contact between higher-order surfaces. The efficacy of the method is demonstrated on several benchmark problems. Continuing and future work is also discussed, with a focus on intended applications and extensions of the method.

Model order reduction for parametrized continuum mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICS GUIDED DATA-DRIVEN MODEL REDUCTION APPLIED TO C02 SEQUESTRATION

Eduardo Gildin[*1], Jungang Chen[1], Daniel Badawi Badawi[1] and Dimitrios Voulanas[1]*

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ABSTRACT

Meeting the net-zero emission paradigm will require a realignment of hydrocarbon production strategies with other forms of energy production (e.g., CCUS, H2, geothermal). Profiting from all these energy sources is only possible if accurate and timely prediction of behavior of fluids, including geomechanics issues in the subsurface, can be attained. Integrated reservoir studies are computationally expensive, especially for performance prediction and decision-making processes. Reduced-order modeling alleviates the computational burden of such simulations by running cheaper and faster models while preserving accuracy. This talk will show the developments of physics-based and Data-driven based proxy models for coupled flow and geomechanics in porous media. We high speedups and accuracy by by introducing several novel components to proxy modeling in porous media: (1) augment the state -space to yield a bi-linear system, and (2) introduce an autoencoder based on deep neural network to linearize physics reservoir equations in a reduced manifold by means of a Koopman operator, and (3) propose a physics-informed convolutional neural network (PICNN) time-varying well controls. While most of PICNNs in existing literatures worked on parameter-to-state mapping, our proposed network parameterizes the solutions with time-varying controls to establish a control-to-state regression. To capture the time-dependent relationship between inputs and outputs, the network is designed to mimic discretized state space equations. We train the network progressively for every time step, enabling it to simultaneously predict oil pressure and water saturation at each timestep. After training the network for one timestep, we leverage transfer learning techniques to expedite the training process for subsequent time step. We will show the performance of this new methodology starting with a small example involving a two-dimensional two-phase (oi and water) reservoir subject to a waterflooding plan with three wells (one injector and two producers). I will also note that our framework is extendable to other studies, especially in the case of CO2 storage processes. Our method achieves speedups of 1000X once properly trained.

Fracture, damage and failure mechanics of cementitious materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADVANCES ON THE USE OF CONDENSED HIGH ASPECT RATIO INTERFACE ELEMENTS TO MODEL COMPRESSIVE FRACTURE IN CONCRETE

Marcela Gimenes[1], Andrei F. V. dos Santos[1], Eduardo A. Rodrigues[1] and Osvaldo L. Manzoli[1]*

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ABSTRACT

The accurate numerical prediction of concrete's failure under compression remains a complex task. Manzoli et al. [1] developed a Mesh Fragmentation Technique in which high aspect ratio interface elements are placed between the regular mesh elements, delineating the potential crack paths. More recently, Gimenes et al. [2] proposed an extension of this technique introducing a two-layer condensed interface element, this duplication is essential for describing compressive failure as a combination of debonding (mode-I) and sliding (mode-II) cracking on the interfaces, which are respectively ruled by tensile and shear-frictional constitutive damage models.

This study showcases the advances on the use of condensed high aspect ratio interface elements to model compressive fracture in concrete. The technique shows suitability for a mesoscale framework, successfully simulating the mesoscale uniaxial compression tests on conventional and recycled aggregate concrete [2] and allowing to understand the influence of each phase (aggregate, mortar matrix and interfacial transition zone) on the material response. In this case, the model can also easily simulate different friction conditions between the concrete specimen and the steel loading plates.

Moreover, on a macroscale framework, the technique suitability is tested to analyze structural size elements such as reinforced concrete beams and compare the different modes of failure associated with the element geometry (span and effective height). In this case, the numerical and experimental [3] results of a four-point bending test are compared, both qualitatively and quantitatively. For the given reinforcement arrangement, the observed failure modes were concrete crush and shear-compression, both were accurately represented using the proposed approach. Besides, the occurrence of two independent damage variable propitiated the assessment of the predominant damage model activated in each beam configuration.

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Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING COMPLEX FLOWS WITH AN OFFLINE-ONLINE DATA-DRIVEN MULTISCALE FRAMEWORK

Juan Marcelo Gimenez[*1], Alessandro Franci[1], Rafael Rangel[1], Eugenio Oñate[1] and Sergio Idelsohn[1]*

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ABSTRACT

The multiscale pseudo-direct numerical simulation (P-DNS) method is a general and efficient framework for the high-fidelity computational simulation of the physics of complex flows [Id20, Gi21, Ide23, Gi24, Ra24]. This data-driven approach is based on four key concepts: i) numerically solving both scales; ii) computing offline fine solutions in representative volume elements (RVEs); iii) storing homogenized responses in dimensionless databases; iv) online solutions at the coarse level and coupling the fine scale via machine learning-based surrogate models. In this presentation, we introduce the latest applications of the P-DNS framework. We study the turbulent particle-laden flow in electrostatic powder coating sprays, the multiphase flow in porous media for CO2 injection processes in geological reservoirs, and the heat transfer through densely packed granular materials. The reliable results obtained with modest resources confirm the potential of the framework as a general approach to build rapid predictive tools in different scenarios.

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AN ADAPTIVE FINITE-ELEMENTS - NEURAL NETWORK METHOD FOR PARAMETRIC PDES

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ABSTRACT

We discuss an adaptive finite-elements neural network method to approximate the solution of a given parametric PDE $F(u(x; \mu)) = 0$, $x \in \Omega$, $\mu \in P$, where Ω and P denote respectively the physical and the parameter spaces. When using neural networks trained with data coming from numerical – in particular finite element – simulations, two main sources of error must be controlled in order to assess the overall accuracy of the method: the error coming from the numerical method that is embedded in the training set, and the error coming from the neural network approximation. More precisely, let ϵ be a given tolerance. Let u_h and u_N denote the finite element and neural network approximations of u respectively and $|||\cdot|||$ be a given norm on $\Omega \times P$. To ensure $|||u - u_N||| \leq \epsilon$, it is sufficient to ask $|||u - u_N||| \leq |||u - u_h||| + |||u_h - u_N||| \leq \epsilon$. The method that we propose to balance the two errors terms uses an adaptive mesh algorithm in order to control the finite element error $|||u - u_h|||$ and adaptively increases the number of training data until the neural network error $|||u_h - u_N|||$ is below the desired tolerance [1, 2]. Numerical experiments will be presented for different model problems, including in particular a Stefan-type problem.

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Novel mathematical and numerical models for multiphysics and multiscale systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PRECONDITIONING THE INCOMPRESSIBLE STOKES PROBLEM WITH VARIABLE VISCOSITY

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ABSTRACT

Incompressible Stokes problem with spatially variable viscosity arises in numerous applications, including geoscience, material science and multi-phase flow. The linear systems resulting from the model are often large, requiring efficient iterative methods for their solution. However, standard block diagonal preconditioners for the Stokes problem perform poorly in the presence of large spatial variations of the viscosity. We address this challenge by conducting a spectral analysis of the Stokes problem. In particular, when the velocity block in the preconditioner is the stiffness matrix/H1-norm, the spectrum of the preconditioned Stokes problem can be fully characterised by the spectrum of the associated Schur complement, which, in the standard case, is preconditioned with the weighted mass matrix for the pressure. We investigate the influence of viscosity distribution on the eigenvalues and the role of eigenvalue distribution on the preconditioner performance. Building upon the spectral analysis, we design block diagonal preconditioners with tailored pressure block that enhances robustness with respect to the viscosity. We finally discuss efficiency of the preconditioner compared to the standard approach.

Scientific machine learning for geophysical applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A DATA-DRIVEN REDUCED ORDER MODEL FOR THE EFFICIENT SIMULATION OF MESOSCALE ATMOSPHERIC FLOW

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ABSTRACT

Despite a continuous increase in computational power, simulations of atmospheric flow using classical discretization methods (e.g., finite element methods or finite volume methods) remain computationally expensive. Given the large number of simulations required to quantify uncertainty in weather prediction, alternatives to such discretization methods are needed to reduce the computational time and allow for improved prediction accuracy in short time frames.

In [1] we focused on the application of three data-driven reduced order models to mesoscale atmospheric flows: DMD, HDMD and PODI. In this work we improve the results presented in [1] by using the POD-LSTM method that exploits special neural network architectures in order to predict the future behaviour of the system at hand.

Our approach is validated in terms of computational time and accuracy in the simulation of two well-known benchmarks for mesoscale flow: the rising thermal bubble and the density current.

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Biomechanics of hard tissues: From experiments and simulations to clinical applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FRACTURE ANALYSIS OF HUMAN VERTEBRA WITH A PHASE FIELD COMPUTATIONAL APPROACH

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ABSTRACT

This study introduces the application of a phase-field model to simulate and analyze fracture patterns, deformation mechanisms, damage, and mechanical responses in a human vertebra following pedicle screw insertion under compressive loading conditions. The proposed phase-field framework effectively captures scenarios where diverse damage patterns, such as crack initiation sites and propagation paths, arise after spinal fusion procedures, considering various simulated physiological movements of the vertebral body. Spatially varying elastic properties and phase-field parameters have been computationally derived from bone density estimations. A convergence analysis was conducted for the vertebra-screws model, employing various mesh refinements, demonstrating consistent agreement with existing literature on this topic. Consequently, by assuming different pedicle screw insertion angles and considering various vertebral motion loading regimes, a comprehensive set of numerical results characterizing damage within the vertebral model has been obtained. Overall, the phase-field findings corroborate and expand upon the current literature, providing valuable insights for the medical community, potentially aiding in enhancing clinical interventions and reducing post-surgical bone failure and screw loosening. Furthermore, the computational approach investigates the effects of fracture and mechanical behaviour of the vertebral-screws system within various metastatic lesions, opening avenues for addressing life-threatening scenarios.

Trustworthy multi-fidelity and data-driven models for computational applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTI-FIDELITY GRAPH U-NET FOR PHYSICS SIMULATIONS

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ABSTRACT

Physics-based deep learning frameworks have shown to be effective in accurately modeling the dynamics of complex physical systems with generalization capability across problem inputs. While unsupervised networks like PINNs rely only on the underlying governing equations and boundary conditions, they are limited in their generalization capabilities. However, data-driven networks like Graph neural networks (GNNs), DeepONets, Neural Operators have proved to be very effective in generalizing the model across unseen domains, resolutions and boundary conditions. But, one of the most critical issues in these data-based models is the computational cost of generating training datasets. Complex phenomena can only be captured accurately using large enough deep networks that require large training datasets. Furthermore, the numerical error of the samples in the training data is propagated in the model errors, which necessitates the need for accurate data, i.e. FEM solutions on high-resolution meshes. Multi-fidelity methods offer a potential solution to reduce the training data requirements and incorporate physics into the neural networks. To this end, we propose a novel GNN architecture called Multi-fidelity Graph U-Net, which incorporates meshes of different granularity at different levels of a graph U-Net architecture and uses outputs from these levels for training the model. We show that this approach performs significantly better in accuracy and data requirement and only requires training of a single network compared to other benchmark multi-fidelity approaches like transfer learning models. Moreover, we observe that this approach requires shallower networks compared to existing GNN models for physics simulations, thus accelerating the training time and reducing the system requirements. We show the results of our approach using two benchmark dataset - mechanical MNIST multi-fidelity data and cantilever beam with varying size and resolutions.

Computational and analytical advances in nonlocal modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ALGEBRAIC MULTIGRID SOLVER FOR NONLOCAL EQUATIONS

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ABSTRACT

The naive discretization of nonlocal operators leads to matrices with significant density, as compared to classical PDE equations. This makes the efficient solution of nonlocal models a challenging task. In this presentation, we will discuss on-going research into hierarchical assembly and algebraic multigrid solution techniques that are suitable for nonlocal models.

Mathematical modeling and simulation for social, environmental, and disaster prevention issues
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A STUDY ON RETROFIT PRIORITY OF PIPES IN SEWER NETWORK BASED ON DISASTER RESILIENCE

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ABSTRACT

In recent years, disasters have become more severe and frequent due to the effects of climate change. There is also a high probability that huge earthquakes such as the Nankai trough earthquake and Tokyo inland earthquake occur within the next few decades. Social infrastructures need to be resilient to such large-scale disasters. In other words, they are required to keep their major functions and to recover quickly after being damaged. In this study, the resilience of a system is quantitatively evaluated using the resilience triangle proposed by MCEER considering the 4Rs, namely, robustness, redundancy, resourcefulness, and rapidity1). We also propose a method to determine the optimal retrofit priority based on resilience evaluation.

A virtual sewer network subjected to large-scale earthquake was selected for the analysis target. The sewer network can be expressed as a directed graph depending on a flow direction, while the nodes and edges represent manholes and sewer pipes respectively. The function of the system is defined as the cumulative flow at the most downstream manhole. The function is decreased when several pipes in the network are damaged and blocked due to a disaster. The resilience of the system can be evaluated from a time series of recovery process of the function obtained through step-by-step emergency restoration to clear the blockages.

It is assumed that seismic retrofitting is conducted on the network in multiple times until all vulnerable pipes are retrofitted. The retrofitted pipes are no longer blocked after a disaster. The resilience of the network after each retrofit phase is given by implementing the restoration simulation. The sum of these resilience values represents effectiveness of the retrofit scenario and can be regarded as the objective function. The optimal retrofit sequence, which minimizes the objective function, was explored using a genetic algorithm as the number of retrofit scenarios is considerably huge.

This study presents a way to quantitatively evaluate the resilience of a sewer network and introduces a method of retrofitting prioritization. It was confirmed that recovery process after a disaster can be precisely understood by handling the system as a network and the result can be useful for evidence-based decision making.

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DOMAIN DECOMPOSITION FOR LARGE NEURAL NETWORKS DESCRIBING BATTERY MECHANICAL RESPONSE

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ABSTRACT

One main challenge related to automotive vehicles is to ensure mechanical safety of battery packs made of thousands of Li-Ion battery cells. During crashes, the cells are subjected to large deformations, which can cause chemical instability. Therefore, one of the main challenges in designing battery cells is to predict their mechanical behavior, while including possible variations in their design, material properties and boundary conditions [1,2]. Simultaneously, we opted to include a probabilistic description of the parameters defining the mechanical behavior, which makes the problem become stochastic. To make the physical model “light-weight”, we design a novel surrogate model that combines domain decomposition methods with deep learning. The idea is to partition the domain into linear and nonlinear regions, and tackle these separately. For this purpose, an alternative minimization method is used, that inherits the objective functions from a classical (or physics-inspired) machine learning setting. The main challenges are the inherit nonlinearity of the problem and the number of parameters describing the networks. For this purpose we will present a novel training approach that takes linearization of the constraints and a reduction of the number of parameters, through a prospective sensitivity analysis, into account. The numerical convergence of the method will be showcased on analytical examples, as well as on the simplified mechanical model of a battery cell.

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Emerging topology and shape optimization techniques in computational design of materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPLICIT MULTI-MATERIAL TOPOLOGY OPTIMIZATION UNDER FINITE DEFORMATION

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ABSTRACT

Advances in additive manufacturing technology have significantly enhanced the capacity to produce structures of diverse shapes with complex configurations. Accordingly, interest in the design of optimized structures increased, leading to active research on topology optimization, an optimization methodology with a high degree of freedom. Topology optimization excels in obtaining optimized structural designs compared to trial-and-error methods. Its effectiveness is particularly notable in designing optimized structures considering multi-materials or -physics, which are challenging to approach intuitively. Multi-material topology optimization offers a broader solution space compared to topology optimization considering only a single material. This wider scope allows access to objective functions that cannot be attained with single-material structures. Therein, multi-material topology optimization has been actively researched across various fields including actuators and biomechanics. However, due to the simplicity of analysis, many existing studies adopted a linear elastic constitutive model; there are limitations to design that encompass finite deformation and hyperelasticity which are typical in real-world applications. Although there are some studies considering structural nonlinearity, there is still a lack of research that quantitatively evaluates the performance improvement of optimized structures by harnessing the synergy among multiple materials with distinctive material nonlinearity.

In addition, to consider the multiple materials and the high-fidelity model considering structural nonlinearity simultaneously, a method that can stably implement finite deformation analysis of intermediate designs while lowering the computational burden is needed. One of the efforts to do so is explicit topology optimization. Recent work by Du et al. [1] considering finite deformation showed that the optimal design could be obtained under a small number of design variables and computational costs through explicit topology optimization.

Therefore, in this study, we present an explicit topology optimization approach for multi-material composite structures, considering both geometric and material nonlinearity. By leveraging synergy among multiple materials with distinctive material nonlinearity, the research presents the quantitative evaluation of the performance improvement of optimized structures under large deformation. Also, the methodology incorporating material nonlinearity into multi-material explicit topology optimization is presented, and the validity of the methodology is demonstrated through numerical examples.

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Geomechanics of the cryosphere
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING SEA ICE IN A WARMING CLIMATE

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ABSTRACT

The precipitous declines of Earth’s sea ice covers are impacting its polar marine environments and their ecosystems, with ripple effects felt far beyond the polar regions. As a material sea ice exhibits composite structure on length scales ranging over many orders of magnitude. From microscale brine inclusions and mesoscale melt ponds, to rich ice pack dynamics on oceanic scales, and from microbes to polar bears, we'll consider recent advances in modeling sea ice and the ecosystems it hosts. With the session focus on new methodologies, we’ll discuss mathematical and computational approaches that we’ve been developing recently to study complex multiscale systems in the cryosphere. These approaches include homogenization for coupling disparate scales in PDE models, fractal analysis, percolation and random matrix theory, topological data analysis, and uncertainty quantification. This work is helping to advance how sea ice is represented in climate models, and to improve projections of the fate of Earth’s sea ice packs and the ecosystems they support.

Modeling and simulation of dynamics, stability and control of aerospace structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RELIABILITY ANALYSIS OF AIRCRAFT WING STRUCTURES BASED ON MONTE CARLO SIMULATION AND FINITE ELEMENT METHOD

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ABSTRACT

As the aerospace industry continues to improve its performance and efficiency, ensuring the structural integrity of aircraft components such as wings is fundamental. Classical deterministic techniques for structural assessment may prove inadequate, given that uncertainties in the system can suppress the actual performance of the aircraft, deviating it from the optimal design [1]. On the other hand, the reliability analysis considers these uncertainties, offering a more robust assessment of the structure's safety, by providing the probability of violating a limit state. In this study, we investigate the reliability of aircraft wing structures. We model wings with different profiles, treating material properties and applied loads as random variables to determine the probability of structural failure and the influence of input parameters on aircraft wing strength. The chosen method of analysis is the Monte Carlo simulation (MCS), which is the safest for evaluating the probability of failure, subjected to the number of simulations and the quality of the pseudo-random number generator [2]. The limit state function is evaluated using finite element method (FEM), carried out in the MATLAB® environment.

Keywords: structural reliability, aerospace structures, Monte Carlo simulation, finite element method.

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NUMERICAL SIMULATIONS OF ORIGAMI-BASED FOLDED CARBON-REINFORCED CONCRETE SHELLS

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ABSTRACT

The advantages of carbon-reinforced concrete (CRC) over traditional concrete elements reinforced with steel, such as high strength, low weight, and corrosion resistance, make it a promising material for thin, efficient, and more sustainable designs. As the demand for less CO2-intensive materials such as concrete grows, a shift from simple massive elements to thin-walled elements with complex geometries is becoming increasingly necessary. However, to seek optimal design variants, efficient nonlinear numerical calculations that provide reasonable predictions of the structural behavior, including the stress-redistribution process and the failure mechanisms are essential. This paper presents FEM simulations of origami-based folded CRC shells that were experimentally investigated in a previous study. Two FEM modeling approaches were employed in the shell numerical analysis, one using a smeared and the other a discrete representation of the carbon reinforcement. Both approaches employed a damage-plastic nonlinear material model for the concrete. The load-deflection response obtained from the discrete approach closely matched the experimentally obtained curves. Despite an overestimation of the load capacity, the computationally less expensive smeared FEM model was able to qualitatively reproduce the structural response and the correct failure mechanism. Alternatively, a multiscale approach was discussed. In this approach, the structural scale is modelled using shell elements, while the reinforcement geometry is represented by NURBS (Non-Uniform Rational B-Spline) surfaces. The quality of the results obtained from the smeared model is sufficient to determine preferred design variants in typical design situations. However, the development of more accurate modeling approaches that are also computationally efficient, such as multiscale methods for shells, is needed to facilitate the sustainable design and application of thin CRC elements in future research contributions.

Computational models and methods for predicting cancer progression and treatment response
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DELTA-P1 MODEL IMPLEMENTATION FOR NUMERICAL SIMULATION OF PHOTOTHERMAL CANCER THERAPY IN THREE-DIMENSIONAL HETEROGENEOUS TISSUES

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ABSTRACT

Photothermal therapy (PTT) stands as a promising avenue for cancer treatment. Pplasmonic gold nanoparticles (GNP) absorb near-infrared light, inducing localized heating for tumor cell apoptosis. Predicting spatial temperature in preclinical models is crucial due to cell death sensitivity to temperature changes. Heat transfer models, particularly those relying on the radiative transport equation (RTE), are essential for this purpose, but their accuracy hinges on suitable approximations for light transport in heterogeneous media with NPs. The Pennes bioheat equation, which describes heat transfer in biological tissues, is known to be highly sensitive to the chosen approximation for the RTE when modeling PTT. Hence, a crucial need arises for a tailored approximation in NP-containing media, especially in irregular tumor geometries. Existing models for RTE has limitations; Beer-Lambert ignores light scattering, P1 is only valid under tissues with low absorption and high scattering coefficients [1], and discrete ordinates and MC simulations can be computationally demanding, particularly in real-time scenarios. This study focuses on the delta-P1 model, a modification of the diffusion approximation proposed by Prahl for biomedical applications [2]. Unlike P1, the delta-P1 model treats forward and scattered light independently, preserving precision across a broader range of optical properties, including media with NPs. Moreover, the model is formulated in three dimensions, allowing straightforward implementation in irregular geometries. The delta-P1 model equations are solved by the Finite Element Method (FEM) within the open-source framework FEniCSx. Numerical results for fluence rate in a heterogeneous geometry with nanoshells is compared to MC simulations and the P1 approximation. Temperature distributions are obtained by numerically solving the Penne’s equation. The delta-P1 model shows a significant improvement over P1 in heat transfer simulations, especially in irregular tumor geometries . Delta-P1 model application to irregular geometries has not been reported . Therefore, this study validates and applies the model for simulating light transport in PTT in general geometries. It shows enhanced accuracy in heat transfer simulations, particularly in scenarios with heterogeneous tissues and GNPs. This underscores its potential as a valuable tool for optimizing PTT preclinical models .

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New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION OF SOLID OXIDE FUEL CELL (SOFC) CHANNELS USING A HYBRID MODELING STRATEGY

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ABSTRACT

There is a growing demand for energy sources that are mainly dependent on fossil fuels nowadays, which are limited resources and have severe environmental impacts. Consequently, energy diversification and the employment of alternative energy sources are becoming even more critical. In this context, the fuel cell is a device that generates energy from electrochemical reactions, which makes it a cleaner and more sustainable alternative to conventional energy conversion technologies [1]. In this work, we apply a methodology based on the topology optimization method to design both the air and fuel channels of a solid oxide fuel cell (SOFC), aiming to improve its electrochemical efficiency. For that, we propose a hybrid modeling strategy that combines a 3D Finite Element (FE) model for the cell electrodes (cathode and anode) and electrolyte with a simplified 2D model to represent the flow behavior and diffusion in the cell channels. The Brinkmann Equations are used to model the momentum balance in the porous electrodes, coupled with the Stefan-Maxwell model to regard the multi-component species transport. Moreover, the Butler-Volmer equation describes the electrochemical reaction at each electrode, which plays a crucial role in modeling the SOFC performance since it drives all other occurring processes [2]. This hybrid modeling approach allows us to have a good representation of the physics involved in the electrolyte and porous electrodes, which is required to analyze the cell performance more precisely. At the same time, the simplified channel model significantly reduces the computational costs, which is also essential when solving a topology optimization problem. The Globally Convergent Method of Moving Asymptotes (GCMMA) is used to update the design variables during the optimization process, and a few design solutions for the cell channels obtained by the proposed methodology are presented.

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Fluid-structure interaction: Methods and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RESEARCH ON CONVERGENCE AND OPTIMAL PARAMETERS OF INERTIAL RELAXED LBM FOR FLUID AND SOLID SIMULATIONS

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ABSTRACT

The handling of boundary conditions in fluid-structure interaction (FSI) is a difficult task. The lattice Boltzmann method (LBM) has been proven to be efficient in processing boundary conditions in fluid simulations, its application is generalized for solid simulations in recent years. However, LBM usually suffers from slow convergence, which limits its applicable scenarios.

To adress this issue, an accelerated LBM suitable for both fluid and solid simulations based on the inertia relaxed Bhatnagar-Gross-Krook operator (BGK-IR) is proposed. Combining the Chapman-Enskog theory and our previous work, the Navier-Stokes equations and the equation of elastic lamina deformation are restored from the BGK-IR, and the Boltzmann equation based on the BGK-IR has a second-order error with respect to the time step and the inertia term.

During numerical tests, the D2Q9 and the D3Q15 lattice velocity models are selected. The elastic lamina, the 2-D square cavity flow and the 3-D cubic cavity flow are selected as simulation objects. Series of numerical are conducted, and the results are compared with the benchmark solution in detail. The results proves that comparing with the original BGK-LBM, BGK-IR-LBM possessed acceptable accuracy and superior convergence rate. Based on optimal parameters, the time consumption in fluid simulation and solid simulation has been reduced by 60.72% and 35.25% respectively.

Our work discusses the application of the BGK-IR operator in fluid and solid simulations for the first time. The superior convergence of BGK-IR-LBM, as well as its applicability for both fluid and solid simulations, are demonstrated. Despite that BGK-IR-LBM incurs ill accuracy as the value of the inertial term becomes large, given its rapid convergence rate, a hybrid algorithm could be developed to restart the calculation process from the relaxed solution and compensate for the lack of calculation accuracy. This is our future work.

Analytical models for nonlinear dynamics and evolved dynamics in natural, social and engineering sciences
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NEW SECONDARY DEFLECTIONS FOR THE FLOW OF PRANDTL-MEYER

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ABSTRACT

A new formulation by components for the deflection of the Prandtl-Meyer flow is applied. For this purpose, the radial and transverse components of the deflection of the flow are recognized through a geometric analysis to complement the classical specialized literature. Typically, through the last decades the deflection was obtained by numerical methods by integrating from an initial state (incident flow) and arriving at the presetting final state (deflected flow). So, the integration in general covers the expansion region. The goal of this paper is to provide access to the infinite intermediate geometry in analytical form and to reach exact, selective and by components procedures and formulations. The contribution to the field of Computational Fluid Dynamics CFD is to facilitate the deeper analysis of the Prandtl-Meyer flow from nonlinear secondary tangential components of the deflected flow.

Modeling and simulation of advanced manufacturing processes for metals
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RESEARCH OF THE SIMULATION ACCURACY OF THE RING RADIAL ROLLING PROCESS

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ABSTRACT

The paper presents the results of research the accuracy of the simulation of the hot rolling process of steel rings. This process involves reducing the cross-section of the pre-formed charge, resulting in rings with relatively large diameters in relation to the cross-sectional dimensions. In numerical simulations of the process, there are problems with obtaining good agreement between the experimental and theoretical dimensions of the product. For this reason, it was considered advisable to perform simulation quality tests using selected commercial programs. The research consisted of carrying out experimental tests of ring rolling with selected process parameters, and then simulating these tests using three commercial computational programs based on the finite element method. Each program uses a special module for ring rolling and a general module. In the first stage, the friction factor was determined taking into account the similarity of theoretical and experimental results regarding the occurrence of the slip phenomenon. In the second stage of the research, the dimensional accuracy of the simulation was determined based on the difference in the internal and external diameters of the rolled rings obtained as a result of the simulation and in the actual rolling process. Based on the results obtained, the advantages and disadvantages of the computer programs used were indicated.

Physical models and reduced order models augmentation with data for physics-informed machine learning in real-world applications
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THERMODYNAMICS-INFORMED GRAPH NEURAL NETWORKS FOR DIGITAL HUMAN TWINS

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ABSTRACT

Key Words: Human Digital Twins, Geometric Deep Learning, learned simulators, Thermodynamics
Numerical simulation has established itself as a fundamental resource in the modelling of the behaviour of physical systems, allowing large-scale calculations to be carried out. However, the emergence of more sophisticated biological models and the need to enhance the performance of these calculations, with a view to more ambitious goals, motivates us to explore alternatives to the traditionally established methods, such as the finite element method (FEM).

Geometric deep learning models [1], based on the thermodynamics of the problem and their ability to identify the dynamics of unknown systems [2], even in the presence of highly nonlinear behaviour, are a promising perspective to address this increasing complexity. Following the line of these learning models, our work aims to validate their applicability to biological systems and to explore the new possibilities that artificial intelligence can offer to this field.

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Complex fluid flows in engineering: Modeling, simulation, and optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL SIMULATION OF THE PHASE-CHANGE EVOLUTION DURING THE STRAND EXTRUSION IN FUSED DEPOSITION MODELING

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ABSTRACT

A numerical study of the phase-change evolution during the extrusion and deposition of a single strand in a fused deposition modeling (FDM) process is carried out. The FDM process is a popular fabrication process mainly used in manufacturing functional parts and rapid prototyping. The numerical framework is based on the stabilized finite-element method and the Arbitrary Lagrangian Eulerian (ALE) formulation. A boundary-conforming approach is used to track the filament motion, allowing an accurate description of the strand shape since the free surface matches exactly the strand boundary [1]. The mesh motion is enhanced by using the surface-reconstruction virtual-region method (SR-VR) [2], which is designed for problems with large mesh translation and topology changes, such as FDM. Furthermore, the SR-VR method allows the extrusion of both mesh and material from the printed nozzle, leading to continuously enlarging the domain over time. The Cross-WLF viscosity model is used to represent the shear thinning and the temperature-dependent behavior of the polymer material.

Our boundary-conforming framework is coupled with a source-based interface-capturing method to follow the phase transition during the process. In particular, the same method is used to track the melting evolution inside the nozzle and the solidification front after the deposition. Thus, the developed framework enables the study of key parts of the process, such as melting, extrusion, deposition, cooling, and solidification, in a single simulation. Results of temperature distribution, phase-change evolution, and strand shape at different process parameters will be presented and discussed.

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Imaging and computational methods for biomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CHARACTERIZATION OF PIG VERTEBRAE UNDER AXIAL COMPRESSION: INTEGRATING RADIOMIC TECHNIQUES AND FINITE ELEMENT ANALYSIS FOR ACCURATE DIAGNOSIS OF SKELETAL SYSTEM DISORDERS

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ABSTRACT

Research on pig bones, given their anatomical similarities to human tissues, has significantly advanced diagnostic tools for the diagnosis of skeletal system disorders. Employing radiomic techniques, medical image segmentation and finite element analysis, we can comprehensively assess bone damage, density loss and mechanical functionality, providing a remarkable advance in personalized medicine. Experimental tests were performed on L3-L6 porcine vertebrae under compression axial loading conditions to analyze their mechanical properties and determine the force response versus displacement and maximum loads in the elastic range. Using computerized axial tomography, we generated three-dimensional models using segmentation techniques and applied anisotropic material models for finite element analysis. The methodology demonstrated strong correlation with experimental data, showing differences of less than 0.8% in elastic modulus and 1.53% in displacement. This approach provides strong support for accurate medical results, using the models as diagnostic references. It also allows to better understand the interactions of implants with the surrounding bone tissue and to guide the design of medical devices for optimal osseointegration and patient healing.

A FINITE ELEMENT BASED UNRESOLVED CFD-DEM METHOD FOR HIGHLY DENSE PARTICLE FLOWS

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ABSTRACT

In this work, we develop a fully coupled fluid-particle interaction algorithm for particle-laden flows. The flow is solved using the Volume Averaged Navier-Stokes equations (VANS), discretized employing Finite Element Method (FEM), and stabilized via the Variational Multiscale (VMS) framework. The Discrete Element Method (DEM) is utilized to track individual particles. The transfer of the information from particle to the continuum consists of a polynomial kernel-based projection that lets us generalize the CFD-DEM to solve problems that require fluid element sizes of the same order as that of the particles.

We show some particularities in our algorithm. First, the transfer of the information from particle to the continuum consists of a polynomial kernel-based projection that lets us generalize the CFD-DEM to solve problems that require fluid element sizes of the same order as that of the particles. Second, to improve the stability of the fluid phase solution, we split the drag force into two parts. We treat the part dependent on the particle’s velocity explicitly and the part dependent on the fluid velocity implicitly as a reaction term.

We present some verification examples demonstrating the conservative properties of the coupling and the algorithm's ability to handle dense and highly dynamic multiphase systems such as fluidized beds.

COMPUTATION OF LEAKY MODES OF MICROSTRUCTURED OPTICAL FIBERS

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ABSTRACT

Many modern microstructured fibers guide light by anti-resonant reflection effects. Such guidance mechanisms are often inherently lossy. The loss can be estimated from leaky modes that satisfy an eigenvalue problem derived from Maxwell equations on the fiber's transverse geometry. Using a discrete mixed eigenproblem with Nedelec finite elements, we solve for the eigenvalues and estimate confinement losses. After describing this methodology, the talk will demonstrate that the certain modeling choices have an outsized influence on computed confinement losses. For example, one can obtain disparate mode confinement loss profiles for the same optical fiber design by changing the outer material properties far away from the guiding core. These sensitivities are then tracked to certain fine scale features in modes. We then design an adaptive scheme for leaky modes. The scheme is able to automatically capture the fine scale features. Results obtained by applying the algorithm to various microstructured optical fibers show its utility.

Emerging frontiers and methods in digital manufacturing: Modeling, simulation, and beyond
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VARIATIONAL MULTISCALE METHOD FOR VOID EVOLUTION AND TRANSPORT IN PROCESS MODELING OF POLYMER MATERIALS

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ABSTRACT

The manufacturing of fibrous composites involves cure cycles under high temperature conditions that initiate cross-linking polymerization in the resin to produce a structurally hard composite. Chemical reactions during curing also produce gaseous constituents result in formation of voids in the cured material. We present an integrated computational method for process modeling in polymer materials, considering the discrete microstructure evolution of the material in the early phase when the resin is still in a viscous liquid form, allowing voids to evolve and migrate together with curing of the material. The mathematical framework comprises of a hierarchically coupled system of partial differential equations, which include (i) the unified compressible-incompressible formulation using Navier-Stokes equations for the velocity and pressure in the two fluids, (ii) the advection-diffusion-reaction equation for the evolution of the concentration of contaminants responsible for void growth, (iii) the level-set equation for the evolution of resin-void interface, and (iv) the Laplace-Young equation for incorporating surface tension jump condition across the interface. The sharp discontinuity in viscosity and density across the interface of the liquid and gaseous phases triggers instabilities in the numerical solution due to the (i) discontinuous flux gradients, (ii) pressure overshoot/ undershoot affecting the coupled velocity field, and (iii) local oscillations arising from the singularity of the signed-distance field function and its gradient in the level-set equation. Additionally, the discontinuous diffusion coefficient and strong discontinuity in the concentration field at the interface causes instability in the solution of the advection-diffusion-reaction equation.

We present a stabilized finite element method, facilitated by the variational multiscale (VMS) method, to address these instabilities without smoothing the material jump or the surface tension effects over the interface. The new method is endowed with discontinuity capturing feature that naturally emerges when fine-scale models are embedded with the surface tension jump terms at the discrete interfaces. In the regions with sharp gradients, these variationally projected fine-scale models augment the stability of the coarse-scale formulation to accurately capture sharply varying solution fields without the need for expensive adaptive remeshings. For advection-diffusion-reaction equation, interface condition is enforced via Lagrange multiplier for which analytical solution is derived by embedding discontinuity capturing fine scale models in coarse scale formulation. The resulting formulation allows for one-way coupling between the concentration equation and the momentum equations. Numerical test cases demonstrating void evolution, migration, shape change, growth, and coalescence during the curing process are presented and validated through carefully designed experiments.

Emerging topology and shape optimization techniques in computational design of materials and structures
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DESIGN OF A STRUCTURAL BATTERY COMPOSITE WITH A BI-CONTINUOUS 2-PHASE MATRIX USING A VIRTUAL TEMPERATURE CONSTRAINED TOPOLOGY OPTIMIZATION

Jonathan Gorman[*1], Reza Pejman[1] and Ahmad Najafi[1]*

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ABSTRACT

Structural Battery Composites (SBC) are an innovative class of materials exhibiting multifunctionality by concurrently resisting stresses and providing energy storage capabilities. SBC's can be used to reduce weight through their integration into structural design elements – for instance in electric vehicles. Previous studies have found optimized designs of SBCs; however, the solutions obtained in these works do not possess bi-continuous material distributions [1]. In these cases, regions of Structural Battery Electrolyte (SBE) do not exhibit full continuity between the electrodes, leading to difficulty in passing current between the terminals.

To establish SBC designs with bi-continuous material distributions, this study adds a virtual temperature constraint to the design framework. Previous works have implemented virtual temperature constraints to restrict enclosed voids or islands of solid material in structural designs [2]. In this technique, each phase of the SBC design will be assigned an artificial thermal conductivity: high conductivity for the SBE and low conductivity for the structural phase. Moreover, the SBE phase will function as a fictitious heat source. At the battery electrode locations, zero temperature Dirichlet Boundary Conditions are applied to allow dissipation of the artificially generated heat. By imposing a constraint on the p-norm of the virtual temperature distribution, an efficient current path within the battery can be delivered.

A multi-objective formulation is used in this design framework via the normalized-normal-constraint method that minimizes the stiffness and maximizes the ionic conductivity of the SBC designs. To improve computational performance, this methodology uses the portable extendable toolkit for scientific computing and message passing interface. Furthermore, the sensitivity analysis is fully analytic and implemented using the adjoint method. The versatility of this new framework is demonstrated through several numerical examples.

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Physics-based data-driven modeling and uncertainty quantification in computational materials science and engineering
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ADVANCED SAMPLING ALGORITHMS FOR ACCELERATING MULTI-FIDELITY INFORMATION FUSION

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ABSTRACT

Assessing the effects of input, parameter, and model uncertainties of high-fidelity simulation models is extremely computationally challenging. Sampling methods based on Monte Carlo become infeasible and surrogate methods may lose fidelity. Multifidelity methods have emerged as a complementary technique that enables one to rely on much fewer evaluations of computationally expensive models with little sacrifice in the accuracy of statistical estimates. These methods work on the basis that ensembles of low-fidelity models and experimental data can be leveraged to accelerate the estimate of the statistics in an unbiased manner. In this talk we describe our latest advances in sampling-based approaches for information fusion. These approaches will explore optimal linear estimators, demonstrating the power of approximate control variates to represent a vast majority of other approaches in the literature. In addition, we will discuss the challenges and opportunities of deploying these tools to outer loop settings such as inverse problems, optimization, and data-driven learning. Specifically, we will describe how the approximate control variate [1] can be generalized to encompass any linear information fusion technique, including the multi-level best linear unbiased estimator [2]. We will also discuss how these techniques can be parameterized and extended to predict multiple outputs so that they can be embedded in extensive outer-loop schemes.

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Modeling and learning of structured dynamical systems
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STRUCTURE-ENFORCING AAA ALGORITHM FOR MECHANICAL SYSTEMS

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ABSTRACT

Learning physics-based reduced-order models from data has been a particularly prominent endeavor in both applied mathematics and mechanics in recent years. The AAA (Adaptive Antoulas-Anderson) algorithm by Nakatsukasa, Sete, and Trefethen has become an established data-driven method for rational approximation, harmoniously blending interpolation and least squares (LS) fitting on a data set composed of frequency-response measurements. The fitted models are linear first-order systems characterized by a barycentric representation of their transfer functions. The main contribution presented here is the extension and adaptation of the AAA algorithm for fitting linear systems with second-order dynamics, perfectly suited for applications to mechanical systems. The main innovations are structured barycentric forms for transfer functions of second-order systems, together with the incorporation of optimization techniques that can cope with the extra parameters encountered (and with the nonlinearity of the least-squares problems to be solved). More precisely, the proposed approaches are iterative in the sense that the dimension of the fitted models increases at each step until a certain accuracy on the available data is achieved. This is accomplished by imposing a set of interpolation conditions with interpolation points chosen in a greedy fashion so that the approximation quality may improve at each step of the iteration. Fixing this interpolation property, the systems' transfer functions are then rewritten in different barycentric forms using different parameterizations. Thereafter, an optimization problem is solved at each step in order to determine viable values for the remaining free parameters. Here, different tools are explored, ranging from standard LS approaches to nonlinear LS methods. Numerical examples include the application of the newly developed methods to established mechanical benchmark models, such as a butterfly gyroscope, an artificial fishtail, a hysteretic plate, and also a bone model.

Advances in computational mechanics for flow-induced vibrations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SIMULATING SOFT CORAL VORTEX-INDUCED VIBRATIONS BY COUPLING A WAKE OSCILLATOR MODEL TO A CO-ROTATIONAL BEAM FINITE ELEMENT FORMULATION

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ABSTRACT

Soft corals sway with the low-frequency swell of surface waves and vibrate at a high frequency due to vortex-induced vibrations. It is hypothesized that these high-frequency vibrations allow the soft-coral colony to intercept more food particles and thus improve its feeding. In this conference talk, we present a simulation workflow to couple a co-rotational beam finite element formulation with a wake-oscillator model and an empirical drag formulation. This workflow allows simulating the low frequency, large amplitude sway of the branched structure and its high frequency response to vortex-induced vibrations. To validate these simulations, we perform water tunnel experiments on 3D-printed idealized coral colony structures. Simulations and experiments are performed for ramified structures with different numbers of branches, and for incrementing reduced velocity. Whereas a cantilevered beam exhibits well-defined and spaced-out lock-in ranges where the frequencies of vibration and of vortex shedding coalesce, a ramified structure with more and more branches exhibits a more and more continuous lock-in over increasing reduced velocity. A ramified structure with many branches possesses natural frequencies close to one another. There is thus always a natural frequency close to the frequency of vortex shedding. Moreover, the natural frequencies of branched structures are unevenly spaced. Single frequency, high amplitude response is observed when vortex shedding occurs in a region of low frequency density, and multimodal, low amplitude response is observed when it occurs in a dense frequency region.
Flexibility allows the coral colony to lower the drag it faces under fluid flow. The vibrational response of the colony allows it to “sweep more water” and encounter more particles. Whereas a beam without branches can maximize this gain in the lock-in region of the second mode, a branched structure smooths out the capture gain over a larger reduced velocity range.
More details of the work can be found in Villié et al. (2024). The code developed in this work is integrated in the open-source co-rotational finite element software ONSAS of Vanzulli and Pérez Zerpa (2023).

Villié, A., Vanzulli Pena, M., Pérez Zerpa, J.M., Vétel, J., Etienne, S., Gosselin F.P. “Modelling vortex-induced vibrations of branched structures by coupling a 3D-corotational frame finite element formulation with wake-oscillators” Journal of Fluids and Structures, Volume 125, 104074, 2024
Vanzulli Pena, M., Pérez Zerpa, J.M., “A co-rotational formulation for quasi-steady aerodynamic nonlinear analysis of frame structures”, Heliyon, Volume 9, Issue 9, September 2023, e19990

Accelerating failure predictions through advances in scientific machine learning and scientific computing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN OPERATOR LEARNING APPROACH FOR BRITLE FRACTURE ANALYSIS

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ABSTRACT

In brittle fracture mechanics, parameters like failure trajectories, potential failure zones, and damage indices play crucial roles. While high-fidelity numerical solvers exist to predict these parameters accurately, they are computationally demanding and require fine crack resolution. Additionally, even small adjustments in domain parameters or material properties necessitate separate simulations. To alleviate this computational burden, there is a need for rapid and adaptable surrogate models. However, the discontinuous nature and intricacy of fracture mechanics pose significant challenges to developing such models. In our research, we introduce a physics-informed variational deep operator network (PI-DeepONet) for brittle fracture analysis. PI-DeepONet is trained to link the initial defect configuration with key variables of interest, such as damage and displacements. Once trained, the network can quickly provide the overall solution for any initial crack configuration and loading conditions in the domain. By incorporating physical principles into the model and enhancing data during training, the surrogate model can accurately handle both interpolation and extrapolation tasks. Given the sensitivity of fracture modeling to variations, our proposed PI-DeepONet, employing a hybrid training approach, demonstrates strong accuracy in predicting relevant quantities. This approach can be readily extended to various dynamic systems with complex behaviors.

Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MACHINE LEARNING-BASED ANOMALY DETECTOR FOR EXTERNAL FLOW

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ABSTRACT

Anomaly detection techniques for fluid flows have a crucial importance in fluids engineering. Recently, various machine learning-based anomaly detection methods for fluid systems have been proposed [1]. Machine learning is a data-driven method, which does not require a detailed mathematical model of the target system. Additionally, it is known to provide better performance in detecting the detail of anomalies such as the size and location compared to conventional methods [2]. For example, a machine learning-based burst detection method has been developed for pipelines [3]. However, there are still remaining issues in the application of data-driven anomaly detection methods to external flows. Most of the studies propose image-based methods but do not assume situations where the images needed for anomaly detection cannot be collected.
Motivated above, the aim of this study is to expand the applicability of anomaly detection methods based on machine learning. Hence, we propose an anomaly detection model to identify deformations of an object based on physical quantities in the flow around the object. Specifically, we build a machine-learning model that predicts object shape from the physical quantities. To demonstrate the performance of the proposed model, we consider a flow around a circular cylinder at the Reynolds number of Re_D=100 and flows around anomalous shapes. We prepare a total of 21 anomalous shapes based on seven different anomalous positions and three different scales, 4, 12, and 20% of the radius. We investigate the dependence on three input information patterns: 1) flow field behind the object, 2) sensor measurement behind the object, and 3) lift and drag coefficients. The results show that three machine-learning models are able to accurately detect anomalous shapes of 12 and 20% of the cylinder radius. On the other hand, we observe that the detection accuracy decreases for anomalies with a 4% radius, depending on the type of input information and the location of anomalies.

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ESTIMATION OF 3D DISTRIBUTIONS OF MECHANICAL PARAMETERS FOR BRIDGE BY THE VEHICLE–BRIDGE INTERACTION SYSTEM IDENTIFICATION METHOD

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ABSTRACT

The Vehicle-Bridge Interaction System Identification (VBISI) method, which estimates mechanical parameters of both the vehicle and the bridge (mass, damping and stiffness), bridge vibration and road unevenness from vehicle-mounted sensor information (vehicle position and vertical acceleration vibration) has been proposed and validated by numerical simulation [1]. Nevertheless, its accuracy in real vehicle-real bridge systems is low and the refinement of the dynamic model is a challenge. The method is an optimisation problem where the mechanical parameters are searched for in order to minimise the residual difference between the estimated road unevenness of the front and rear wheels. Numerical simulations of the VBI are carried out for each candidate value of the mechanical parameters to estimate the road surface irregularity. Calculating the loss function for the VBISI method requires performing a VBI simulation based on the estimated parameters, so the computational cost of the parameter exploration process increases rapidly when detailed bridge 3D models are introduced into the simulation. Therefore, a 3D modelling scheme for bridges that can be calculated with high accuracy while reducing the computational load is needed. This study employs Higher-order Hermite family Conforming (HHC) finite elements and incorporates generalised three-variable plate theory to realise a bridge model that retains accuracy while constraining computational expenses. It is confirmed that the VBISI method is capable of estimating the three-dimensional distribution of bridge parameters using this model.

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Modeling and simulation of coupled processes in geological media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SPACE-TIME ANALYSIS FOR THE CONTAINER PROBLEM

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ABSTRACT

The container problem describes the behavior of elastic porous media in a rectangular container, which is completely saturated by an ideal incompressible liquid. Displacement and velocity at the bottom are zero. Motion is possible only in the vertical direction. The top load starts with zero at the beginning and increases to its maximum at the end of duration T. By time the liquid extrudes on the surface of the container while the stress moves to the shrinking elastic solid due to its compression [1]. Space and time gradients are zero in the beginning, the time gradient is zero at the end of duration T also.

The analysis bases on a space-time potential that contains a linear elastic term, a darcy flow term, and a boundary load term [2], [3]. The variation of the potential results in a space-time principle leading to overall equilibrium. The boundary load on the top covers the elastic top load and the pressure difference between top and bottom. Realistically its time gradient is zero in the beginning and zero at the end of duration T.
Quadratic approximation of the displacement in space results in linear elastic stress distribution and cubic liquid pressure distribution. It fulfills compatibility of displacement, strain, and velocity. The cubic approximation of the displacement in time starts with a time gradient of zero and ends after the duration T with a time gradient of zero. Displacements and velocities are zero in the beginning.
The state at the end of duration T results from the minimum of virtual worktime which is the integral of virtual work over space and time. For T towards infinity solutions are available for low order approximation according to the rule of Bernoulli L' Hospital.
The potential decreases for higher order approximation which indicates convergence.

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Continuum biomechanics of active systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ACTIVE MEMBRANE RESPONSE OF THE BAT WING

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ABSTRACT

Birds, bats, and insects have evolved unique wing structures to achieve a wide range of flight capabilities. The compliant skin of the wing distinguishes bats from all other flying animals, and contributes to the remarkable, highly maneuverable flight performance and high energetic efficiency. The structural and functional complexity of the bat wing skin is one of the least understood although important elements of the bat flight anatomy. The wing skin has two unusual features: a discrete array of very soft elastin fibers, and a discrete array of skeletal muscle fibers. The latter is intriguing because skeletal muscle is typically attached to bone, so the arrangement of intramembranous muscle in a soft skin raises questions about its role in flight. In this presentation, a multiscale chemo-mechanical constitutive model for bat wing skin is developed. The chemo-mechanical model links crossbridge cycling to a structure-based continuum model that describes the active viscoelastic behavior of the soft anisotropic skin tissue. A computational approach is employed to investigate the effect of membrane muscle activation on wing deformation and aerodynamic performance. Specifically, results are presented that quantify for the first time: i) the influence of in-plane kinematic motion on the fluid-structure interactions of the wing, ii) the effect of wing muscle activation on the 3D shape conformations of the wing and the resulting aerodynamic performance, and iii) the role of trailing edge muscle activation on wing aeromechanics and aerodynamic performance.

Numerical modeling of granular and multiphase flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOWARDS SIMULATIONS OF INDUSTRIAL GRANULAR MATERIAL PROCESSING USING GPU COMPUTING

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ABSTRACT

Particle shape plays a crucial role in the resulting macroscopic behavior of granular material yet the majority of DEM simulations use simple spheres with non-physical constructs such as rolling friction without fully understanding the implications thereof. While there have been shape studies using super quadric's and ellipsoids over the years, they still have the same single point contact resolution as spheres. The majority of industrially relevant granular materials are however non-curve linear and have shapes that are best captured by polyhedral shapes. Apart from mechanical behavior, thermal conduction as well as cohesion between these particles occurs over a finite-contact area that is more faithfully captured by polyhedra. In this talk the role of particle shape will be explored for a number of industrial cases such as mills, screw feeders and silos along with prescriptions for when shape and size simplifications can be used. The underlying theme of the talk will be on the use of GPU computing in the past decade to advance the physics fidelity of DEM simulations along with reduced run-times. Finally an outlook to the future of using high fidelity DEM to generate data for statistical models and physics informed neural networks that can provide answers in the age of digital twins will be presented.

Modeling and simulation of coupled processes in geological media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

REDUCED ORDER GEOMECHANICS MODELS

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ABSTRACT

Simulation of geomechanics problems is often extremely time consuming as they must span multiple spatial and temporal length scales, often include nonlinearities, and coupled processing. As a result, it is challenging to apply such models in real time scenarios and to calibration or optimization processes which require many model executions. Reduce Order Models (ROM) are fast and accurate (ideally) models trained from computationally complex Full Order Models (FOM), in this case large finite element method simulations of coupled processes. This presentation will discuss the pros and cons for the two dominant types of ROMs, intrusive and non-intrusive. ROM construction and training of parameterized ROM, in which injection rate and material parameters are variable inputs will be discussed. The construction of intrusive ROM for porous media flow, poro-elasticity and poro-elasto-plasticity will be discussed, specifically the challenges associated with non-linear problems. The selection of hyper-parameters, such as the number of modes and the number of sampling points, will be discussed. Lastly, performance of ROM vs FOM presented, where it will be shown that relative performance of the ROM over the FOM increases with the complexity (cost) of the FOM – speed-up of more than 1000 times are possible when the FOM exceeds 100,000 degrees of freedom.

Certification of simulations and model adaptation in computational science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN EQUILIBRATED FLUX A POSTERIORI ERROR ESTIMATOR FOR ADAPTIVE REFINEMENT IN DEFEATURING PROBLEMS

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ABSTRACT

An adaptive refinement strategy, based on an equilibrated flux a posteriori error estimator, is proposed in the context of defeaturing problems. Defeaturing consists in the simplification of a geometry by removing features that are considered not relevant for the approximation of the solution of a given PDE. The proposed adaptive strategy is twofold, accounting both for standard mesh refinement and geometrical refinement, which consists in choosing, at each step, which features need to be included into the geometry in order to significantly increase the accuracy of the solution. With respect to other estimators that were previously proposed in the context of defeaturing, the use of an equilibrated flux reconstruction has two main advantages [1]: first of all, it allows to sharply bound the numerical component of the error on the totally defeatured domain, and secondly, it allows to avoid the evaluation of the normal trace of the numerical flux on the boundary of features. This makes the estimator and the adaptive strategy particularly well-suited for finite element discretizations, in which the numerical flux is typically discontinuous across element edges. The inclusion of the features during the adaptive process is tackled by a cutfem strategy, in order to never remesh the computational domain as the features are added. The estimator then also accounts for the error committed by weakly imposing the boundary conditions on the boundary of the added features.

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MODES OF PT-SYMMETRIC FIBERS WITH GAIN AND LOSS

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ABSTRACT

We model a dielectric optical fiber whose transverse cross section has a lossy core and a gain-medium core, both placed symmetrically about a transverse coordinate axis. The balanced gain and loss mediums are placed to achieve parity time-reversal symmetry (PT symmetry). Non-Hermitian physics of PT symmetric models have gained substantial interest in recent years and there have been many studies into breaking thresholds and exceptional points of analytically solvable models. Our non-Hermitian PT symmetric model generates spectra which cannot be solved analytically. For computing the modes of the fiber and efficiently tracking its changes with respect to some parameters, we utilize the FEAST algorithm. We find a rich variety of exceptional points, re-entrant PT symmetric phases, and a non-monotonic dependence of the PT symmetry breaking threshold on the system parameters. In addition, we investigate spectral variations with respect to angular and distance perturbations in the placement of cores.

PHYSICS-AWARE DEEP AUTOENCODERS FOR MODEL ORDER REDUCTION

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ABSTRACT

To capture the dynamics of systems whose intrinsic solution space does not fall into a linear subspace with a small dimension, nonlinear model order reduction techniques are essential. Compression of the full-order model into a computationally more tractable reduced-order model presents challenges to traditional ROM techniques. Recently, deep autoencoders have gained popularity for their ability to learn a lower-dimensional latent representation of the original full-order manifold where the nonlinear dynamics evolves. However, "off-the-shelf" autoencoders are often purely data-driven and simply learn input-output mappings between statistical distributions. Hence, the majority of these autoencoders ignore the underlying physics priors by failing to preserve the geometry and topology of the nonlinear dynamics manifold, which carry fundamental information about the global behavior of the associated dynamical system.

In this work, we explore several autoencoder-based model reduction strategies to bridge the gap between state-of-the-art deep learning research and the domain-specific needs for reduced-order modeling. We achieve this by quantitatively comparing two categories of physics priors: i) learning bias priors to preserve geometric properties of the dynamics manifold; and ii) inductive bias priors to preserve topological properties of the manifold. In particular, we investigate the performance improvement in autoencoder-based ROMs when they are regularized with an isometry distortion measure, introduced in Lee et al. [1], which captures the induced change in the Riemannian metric, i.e., the intrinsic notion of local length and angles, over the nonlinear dynamics manifold. The conformally-constrained encoder and decoder of this class of models prevent arbitrary change in the amplitude and direction of the infinitesimal dynamics of the physical system when encapsulated into the latent space. In addition, we investigate two inductive bias methods, namely PARC [2] and LaSDI [3], which preserve the topology of the manifold by constraining the flow of the underlying dynamical system. Through these experiments, we compare different design and training schemes for autoencoder-based ROMs and underline the remaining challenges.

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Trustworthy multi-fidelity and data-driven models for computational applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOWARDS TRUSTWORTHINESS THROUGH THE LENS OF GEOMETRIC INTERPRETATION

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ABSTRACT

High-dimensional parameter spaces present a dilemma for the current state-of-the-art AI models: we have limited analytical foundations for understanding and quantifying the reliability of these methods despite an apparent usefulness of the models in applications. Common intuitions break down in high dimensions (no such thing a nearest neighbor!) and numerical methods are complicated by implicit biases related to multiple model-fidelity along with a lapse in trustworthiness of extrapolation and interpolation. This work emphasizes geometric strategies for inferring intrinsic dimensionality and systematic parameter dimension reduction to resolve this impasse. We will explore arguments for improved understanding and trustworthiness of AI/ML technologies through well-posed notions of between-ness (distance) and reduced dimensionality---facilitated by principled interpretations and explanations of an applied geometry.

Physics-based data-driven modeling and uncertainty quantification in computational materials science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-BASED ESTIMATES OF EXTREMES OF RANDOM FUNCTIONS

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ABSTRACT

The safe design of, e.g., flood protection systems, aircrafts and high-rise buildings, requires accurate estimates of extremes of river flows, aerodynamic forces and other random functions. The characterization of extremes of random functions is challenging since they require detailed information on these functions which is rarely available in applications. To overcome these difficulties, we construct finite dimensional (FD) models, i.e., deterministic functions of time and a finite set of d random variables, fit them to the available information and show that they can be used as surrogates under some conditions.

Let $X(t)$ be a stochastic process defined on a time interval $[0,\tau]$, e.g., τ can be the duration of a wind storm acting on a building and suppose that the information on this process consists of n sample paths $x_i(t)$, $i=1,\ldots,n$, of this process. Our objective is to estimate the distribution of the extreme X_τ of this process in $[0,\tau]$. Generally, the data set is insufficient to estimate the distribution of X_τ. The following three-step algorithm is used for solution. First, an FD model $X_d(t)=\sum_{k=1}^d Z_k\,\varphi_k(t)$ is constructed for $X(t)$, where $\{\varphi_k\}$ are basis functions and $\{Z_k\}$ are random coefficients. For example, $\{\varphi_k\}$ and $\{Z_k\}$ can be eigenfunctions of the correlation function of $X(t)$ and projections of the realization of $X(t)$ on these functions. Second, an extension of the polynomial chaos (PC) representation, referred to as PCT, is used to construct the joint distribution of $\{Z_k\}$. This distribution and the expression of $X_d(t)$ are used to generate an infinite supply of FD sample paths. Third, conditions are established under which the distribution of the extreme $X_{d,\tau}$ of $X_d(t)$ in $[0,\tau]$ converges to that of X_τ so that FD paths can be used to estimate the latter distribution. Wind pressure time series recorded at the boundary layer wind tunnel facility at the University of Florida are used to illustrate the implementation and assess the performance of the algorithm.

Geometric mechanics formulations and structure-preserving discretizations for continuum mechanics and kinetic models
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LEARNING METRIPLECTIC SYSTEMS FROM FULL AND PARTIAL STATE INFORMATION

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ABSTRACT

A method is presented for learning metriplectic systems from data which is energy-conserving and entropy stable by construction. In addition to respecting metriplecticity, this method comes with approximation results demonstrating its ability to learn general metriplectic dynamics as well as an error estimate indicating its generalization to unseen timescales. Examples are provided which illustrate the performance of this approach in the presence of both full state information as well as when entropic variables are unknown.

Efficient numerical methods for CFD and FSI simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPARING PRECONDITIONING STRATEGIES FOR THE IMPLICIT FORMULATION OF THE IMMERSED BOUNDARY METHOD

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ABSTRACT

The Immersed Boundary (IB) method represents a straightforward and adaptable computational strategy for simulating fluid-structure interaction. Despite its flexibility, the IB method encounters significant timestep size limitations when applied to modeling stiff structures. Fully implicit formulations of the IB method remove the severe timestep size restriction posed by the explicit formulation; however, the linear system derived from the implicit formulation of the IB method proves challenging to solve iteratively without the support of an effective preconditioner. In this context, we introduce and analyze several novel preconditioning strategies designed to enhance the efficiency of implicit formulations of the IB method. We apply our preconditioning strategies to a number of model and application based problems and demonstrate a marked increase in computational speed, offering a compelling alternative to traditional explicit timestepping schemes.

Catastrophic failure mechanics and numerical modelling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ORDINARY STATE-BASED PERIDYNAMIC HYGRO-MECHANICAL COUPLED MODEL FOR MOISTURE DIFFUSION AND CURLING ANALYSIS IN SOIL DESICCATION

Xin Gu[*1], Panyong Liu[1], Yang Lu[1], Xiaozhou Xia[1], Lei Wang[1], Erdogan Madenci[2] and Qing Zhang[1]*

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ABSTRACT

Soil curling is a natural phenomenon in thin soil fragments induced by desiccation cracks, and it further increases the potential threats of soil cracking. When analyzing soil curling especially together with soil desiccation cracking, the existing numerical investigations usually encounter challenges arising from various factors, e.g., inadequate knowledge of soil curling mechanism, complex soil characteristics with diverse parameters, moving boundary conditions during deformation, and crack initiation and growth. Therefore, the present study attempts to reveal the soil curling mechanism through a fully coupled hygro-mechanical ordinary state-based peridynamic (OSB PD) model and corresponding solutions. Specifically, the PD form of the moisture diffusion equations for saturated and unsaturated states are derived by employing the Hamiltonian principle with nonconservative Lagrangian action and peridynamic differential operator (PDDO). Also, the PD bond force is derived by considering the energy equivalent principle for a fully coupled hygro-mechanical model. For the numerical implementation, both staggered and monolithic schemes are developed for the coupled hygro-mechanical problem. The method of controlling the maximum number of bond breakage for non-convergence is explored in the monolithic scheme as well.

A model of soil strip desiccation deformation and curling is constructed while considering realistic moving boundaries of moisture and displacement with relevant parameters, and soil characteristics evolution from saturated to unsaturated states. This model successfully captures the entire curling process, including concave-up and concave-down curling. Also, the influence factors of liquid limit, extra evaporation surface, and thickness on the curling performance are explored. Summarily, the coupled hygro-mechanical peridynamic model provides a potential strategy in soil desiccation cracking investigation for real-scale simulation and fine mechanism exploration.

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Scientific machine learning for geophysical applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOWARD THE REALISATION OF AN ACTIVE FAULT DIGITAL TWIN TO MONITOR SLOW EARTHQUAKES

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ABSTRACT

The discovery of slow earthquakes has revolutionised our understanding of fault friction and of the seismic cycle. Slow slip events (SSEs) play an important role in the seismic budget calculation, releasing equivalent magnitudes even larger than M7. SSEs can be seen as regular earthquakes in slow motion. They do not radiate seismic waves because they are too slow, but they can trigger large (M>7) destructive earthquakes. Therefore, we need to accurately model them if we want to better assess the seismic hazard of seismogenetic structures. We will present the results of a near real-time procedure to retrieve the spatio-temporal evolution of slow earthquakes. To achieve this goal, we use daily sampled Global Navigation Satellite System (GNSS) position time series retrieved in the Cascadia subduction area. This region is ideal because of the high number of major slow earthquake recurrences, and the high density of geodetic stations. The automatic procedure to extract the tectonic contribution from the geodetic observations is based on a variational Bayesian Independent Component Analysis (vbICA) method, an unsupervised learning approach rooted in multivariate statistics that allows us to disentangle the tectonic signal from other sources of deformation (e.g., due to hydrological load). We use the version of the algorithm adapted to handle missing data, a common issue with geophysical observations [2]. The selection of the Independent Components (ICs) is automatised based on the power spectrum of their temporal evolution as well as the coherence of the corresponding spatial distribution. The slip distribution on the fault, regularly updated with the incoming of new data, will be used to determine the temporal evolution of relevant dynamical quantities like the system’s dimension [3], and it constitutes the first step to attempt the forecast of slow earthquakes in near real-time.

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STRUCTURE-PRESERVING INTEGRATION FOR NONLINEAR VISCOELASTODYNAMICS

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ABSTRACT

Numerous polymeric and biological materials may undergo large deformation with intrinsic viscous dissipative mechanisms. Achieving accurate simulations of their mechanical behaviors requires stable and accurate time integration schemes. Traditional time integration schemes are prone to lose stability when applied to nonlinear systems, resulting in a pathological growth of the total energy. Extensive research has indicated that structure-preserving integrators enjoy superior robustness and accuracy in long-term simulation of nonlinear problems, and this leads to a growing interest in the design of such type of integrators.

In this presentation, we will introduce a structure-preserving integrator designed for finite viscoelasticity models[1] constructed within a concrete thermomechanical framework. It can be viewed as a theory built based on the kinematic assumption introduced by Green & Naghdi and generalized by Miehe[2]. Additionally, we also introduce a two-parameter family of nonlinear strain measures, which accurately describe material behaviors over a wide range of deformation states. The numerical schemes are developed using the following critical techniques[3]. Firstly, a velocity-pressure mixed formulation is utilized, which allows the introduction of a new Hamiltonian for fully incompressible materials. We mention that this type of Hamiltonian is different from existing ones in the literature. Secondly, a smooth generalization of the Taylor-Hood element based on NURBS is adopted to construct the semi-discrete formulation, which is inf-sup stable and robust for large-strain analysis. Thirdly, we propose strain-driven constitutive integration formulas for the viscous flow rule, which facilitates the design of the final scheme. Fourthly, the discrete gradient method is applied to devise the time marching scheme for the overall system, with the directionality property extended for inelastic problems. We will present numerical examples to justify the claimed properties of the proposed methods.

Complex fluid flows in engineering: Modeling, simulation, and optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXTENDED DVM ALGORITHM AND TOPOLOGY OPTIMIZATION OF RAREFIED GAS THROUGH A DISCRETE ADJOINT SYSTEM

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ABSTRACT

In this study we present a topology optimization method for rarefied gas flows. The discrete velocity method (DVM) is used to solve the Shakhov kinetic equations, which is a substitution of the Boltzmann equation for modelling rarefied gas flows. The widely-used density method is applied to characterize material distribution in the computational domain, where we develop an extension to the Shakhov equation by modifying the convection term. The extension is continuous with respect to the pseudo design density, and accurately captures the flow conditions in a domain where solid and fluid are mixed. The model topology optimization problem is presented in discretized form, where the discrete numerical variables in DVM are treated as state variables, and the steady state condition of the flow is represented by the zero of a flow residual function. Sensitivity analysis is conducted by considering local linearization of the flow residual, where simple derivations lead us to a discrete adjoint equation. The discrete adjoint equation can be treated as a linear system of equations, where the flux Jacobian of the primal problem is transposed. We argue that the adjoint system can be solved using iterative methods such as the lower-upper symmetric Gauss-Seidel (LU-SGS) method, in a similar way as the primal problem is solved. Gradient-based methods can be used to find the optimal design of flow structures according to the sensitivity obtained from the adjoint system. Numerical examples are provided to demonstrate the validity of the extension of Shakhov equation, the obtained adjoint sensitivity, as well as the topology optimization results.
This study presents a more efficient approach to topology optimization of rarefied flow. Compared to existing approaches [1,2], the present study simplifies the cumbersome derivation of continuous adjoint system, and speeds up convergence due to the use of implicit time-marching schemes. The adjoint system is developed at the steady state of the deterministic numerical approach, hence there is no need to record intermediate results, which lifts the burden in computer memory. We expect this method to be widely used for design problems in rarefied gas dynamics.

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Advanced numerical methods for the modeling and optimization of coupled dynamical systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MULTI-BODY DYNAMIC MODEL WITH COUPLED RIGIDITY, FLEXIBILITY AND LUBRICATING FOR THE EVALUATION OF THE VIBRATION PERFORMANCE FOR THE PISTON ENGINE

Nanxiang Guan[*1], Yongpeng Gu[1], Zhifeng Xie[1] and Min Zhou[1]*

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ABSTRACT

The piston engine is one of the main power machinery in the world. It outputs power by means of the reciprocating motion of the piston. The development of piston engines tends toward high speed and high power density. However, high-order reciprocating inertial force will become an important excitation source of vibration and noise with increasing the piston speed. The key technology for vibration reduction is how to design a compact structure and maximize balancing the multi-order reciprocating inertial force in the limited space. Hence, based on studying the theory of reciprocating motion and balancing technology of piston engine, we propose an accurate calculation method of high-order inertial load, and establishes a multi-body dynamic model with coupled rigidity, flexibility and lubricating for the evaluation of the vibration performance of a piston engine.

According to the results of modal experiment, the flexible body model with the body, crankshaft and support frame is established based on modeling the connecting rod and piston with rigid bodies; meanwhile, the model for oil film lubricated bearing is established by using Reynolds equations. The rigid-flexible coupling model of the whole engine and the discrete Reynolds equation for hydrodynamic lubrication are fully coupled for solutions. The results of vibration acceleration from the simulation and the test are well conformed. It is proved that the engine model and calculation method is reliable. And a numerical verification method for the vibration performance evaluation of the modified engine balance mechanism and the development of new engines is provided.

WAVE PROPAGATION SIMULATION FOR COUPLE STRESS ELASTODYNAMICS USING MIXED FINITE ELEMENT METHODS

José Ortiz-Ocampo[1] and Nicolás Guarín-Zapata[1]*

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ABSTRACT

In recent years, there has been a growing interest in architected materials and the exploration of microstructural interactions and their influence on the macroscopic properties of continuum media [1]. These interactions go beyond classical continuum mechanics models, prompting researchers to propose non-classical models with additional parameters to capture these effects. One such model is couple stress theory, which incorporates microstructural effects through a generalization of Cauchy's postulate, introducing additional mechanical interactions involving couples per unit surface or couple-stresses [2]. However, these models result in higher-order partial differential equations, requiring higher continuity formulations of the Finite Element Methods [3]. To overcome this problem, this work presents a mixed finite element formulation for wave propagation in the time domain. It allows the direct simulation of oscillatory phenomena where the dispersive behavior of waves is presented and the computation of bulk properties for heterogeneous materials.

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Advance modeling and simulation in complex porous media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATION OF RADIAL BASIS FUNCTIONS IN AN IMMERSED BOUNDARY METHOD FOR PARALLEL CFD SIMULATION

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ABSTRACT

Using Computational Fluid Dynamics (CFD) to predict flow and reactions in complex porous media is becoming increasingly feasible, but computing costs still limit the cases that can be tackled. Large (real) domain sizes, high Reynolds numbers, and wide ranges of pore scales affect both the memory and computing efforts required to make accurate and useful predictions. An approach to conduct real-scale simulations in porous media is the use of adaptive mesh refinement (AMR), which allows for the capture of rich and complex gradients in pressure and velocity fields that often occur in porous media. In this context, AMR is challenging because it requires constant remeshing while maintaining the topology of the porous media. Furthermore, this challenge is exacerbated when hexahedral meshes are used.

This work focuses on the implementation, verification, and validation of a method based on Radial Basis Functions (RBF) networks to represent any geometry, enabling the application of Immersed Boundary (IB) conditions within complex porous media. IB methods alleviate the challenges of building conformal grids and enable the use of Cartesian grids, whose simplicity and efficient data structures allow for dynamic AMR during solver execution.

The RBF-based representation of porous media for IB imposition is performed in the Finite Element (FE) solver Lethe, which is based on deal.II. The solver takes advantage of Cartesian hierarchical grids to solve massively parallel simulations on distributed architectures. Building on the same idea, RBF networks use compactly supported basis functions that are distributed among parallel processes while preserving ease of evaluation. The verification of arbitrary feature-capturing capabilities is done using the Method of Manufactured Solutions (MMS), with analytical solutions tailored to verify the flow around the given shapes. The solver is validated by comparing the pressure drop within centimeter-scale porous monoliths (100 to 300 microns pore size) digitized by X-ray microtomography, for Reynolds numbers up to 1000.

The presentation emphasizes on RBF network training and optimization in a parallel framework. The algorithms for the initialization and distribution of the RBF nodes among the processes are covered, as well as the MMS formulation and validation setup. The presentation demonstrates that RBF networks are a light, versatile, and powerful method to represent porous media in pore-resolved simulations, especially when IB methods are involved.

Emerging topology and shape optimization techniques in computational design of materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CONTROLLING DAMAGE - OPTIMIZATION BASED ON ANALYTICAL GRADIENTS AND APPLICATION IN FORMING

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ABSTRACT

Decrease of material usage under the same operative load calls for application of tight tolerances to manufactured parts within the industrial setting. This in return requires a more detailed description of the material models used to simulate a manufacturing process. While plasticity is incorporated in most simulations and many optimization environments, the aspect of damage evolution and accumulation is another important effect to consider. Within the field of optimization, consideration of ductile damage is a scarcely researched topic. However, inclusion of damage modelling enables optimization of processes, such that damage can be reduced and therefore failure of a part under operative load can be prevented.

Introduction of damage mechanics within simulations comes with additional challenges, such as the inherent mesh-dependency of standard local damage models. Gradient-enhanced, non-local damage models have the advantage of mesh-independency, but introduce an additional global damage variable to the problem and require long computation times. Derivation of the gradients for gradient-based optimization also requires handling of internal history variables and its numerical implementation [1]. However, when derived and implemented, these analytically derived gradients are very efficient. For industrial applications, like forming, however, the inclusion of contact mechanics adds another difficulty to optimization. Derivation of analytical gradients for a discontinuous problem is very complex. To circumvent this problem, an optimization framework around a commercial FEM solver is derived. The finite element simulation, with the troubling contact mechanics, is handled within the commercial software, and an optimization environment is structured around this software. This allows damage optimization of forming processes [2].
This talk presents an overview of damage optimization in two fields of research. In the first field, a non-local, ductile damage model is enhanced with sensitivity analysis by a variational approach. The analytically derived gradients are applied within gradient-based optimization and enables creation of damage tolerant structures. The second field of research aims to directly optimize forming processes. This is achieved by creating a framework around the simulation software Abaqus and enables direct optimization for forming processes like extrusion and deep-drawing. Solutions of the optimization problems are optimal process parameters, which correlate with reduced damage accumulation.

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Nanomechanics and nanoscale thermal transport for new materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE EFFECT OF TEMPERATURE AND WATER CONTENT ON THE MECHANICAL PROPERTIES OF NA-MMT UNDER UNIAXIAL COMPRESSION: MOLECULAR DYNAMICS SIMULATIONS

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ABSTRACT

Sodium montmorillonite (Na-MMT) is the main active mineral in clays. It is very sensitive to changes in temperature and degree of hydration. Meanwhile, montmorillonite is characterized by wide distribution, low permeability and high adsorption capacity. It is a potential nano-adsorbent, a nanofiller for polymer nanocomposites, and a basic material for engineered barriers for nuclear waste disposal. However, studies at the microscopic level are insufficient to fully investigate the coupling effects of temperature and water content on the structural properties of Na-MMT. In this study, a molecular dynamics (MD) approach was used to simulate the structure and microscopic mechanical properties of Na-MMT. The aim of this study is to investigate the effects of different temperatures (200 K to 600 K) and water contents (10%, 20% and 30%) on the mechanical properties of Na-MMT. Parameters such as van der Waals force, energy, elastic modulus, shear modulus, bulk modulus and Poisson's ratio were compared. The simulation results reveal several important findings: (1) The behavior and motion of water molecules are significantly affected by the temperature increase, which leads to interlayer expansion and thus reduces the mechanical properties. (2) Na-MMT exhibits anisotropy, with higher mechanical properties in the Y-direction than in the X- and Z-directions as temperature and temperature increase, and the overall ultimate stress shows a decreasing trend. (3) Damage induced by temperature and hydration level is most likely to occur in the Z-direction. The increase in the number of water molecules between the layers and the diffusion due to temperature resulted in a significant weakening of the interlayer van der Waals forces. The results of this study contribute to a deeper understanding of the microscopic characteristics of Na-MMT and provide ideas for the microstructural changes behind the swelling mechanism of bentonite.

16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Advancements in model reduction, data assimilation, and uncertainty quantification for complex physical systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NONLINEAR REDUCED MODELS FOR PARAMETRIC PDES

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ABSTRACT

Reduced order modeling is a powerful tool for approximating the solution to parametric/random partial differential equations. The usual approach is to construct one linear space which accurately approximates the parameter-to-solution map, and then use it to build an efficient forward solver. However, such approach is not suitable for problems with slowly decaying Kolmogorov n-width (e.g., convection-dominated problems) as they would require using a linear space of high dimension. For such problems, nonlinear reduced models present an attractive alternative. In a so-called library approximation, the idea is to replace the single linear space by a collection of affine spaces of small dimension and then use, for any given parameter, the appropriate space in the library. In this presentation, we introduce new algorithms for generating such libraries and illustrate their performances on several numerical examples.

Constitutive modeling of complex materials with machine learning and artificial intelligence
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CONCURRENT MULTISCALE SIMULATIONS OF NONLINEAR RANDOM MATERIALS: A PROBABILISTIC LEARNING PERSPECTIVE

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ABSTRACT

In this work, we focus on the construction of statistical surrogates for concurrent multiscale modeling in structures comprising nonlinear random materials. We specifically address the case of highly stochastic, highly nonlinear (and potentially, non-local) homogenized constitutive models, and use probabilistic learning to approximate the mapping between deformation and stress variables. The approximation problem is formulated using conditional statistics, and probabilistic learning on manifolds is used to draw samples of the nonlinear constitutive model at mesoscale. Two applications, relevant to inverse problem solving and forward propagation, are presented in the context of nonlinear elasticity. It is shown that the proposed framework enables accurate predictions, despite the small data regime and the very high levels of nonlinearity and stochasticity exhibited by the system.

Mesh-free particle methods for multi-physics problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INFLUENCE OF CAVITY PARTITION ON THE DAMPING PERFORMANCE OF ADDITIVELY MANUFACTURED PARTICLE DAMPERS

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ABSTRACT

Particle damping is an effective passive method of vibration suppression. The remarkable advantages of particle damper, such as insensitivity to ambient temperature and availability at a wide range of frequencies, make it available for various applications [1]. However, a limitation for applying traditional particle damper is that an additional installation space is needed.

Additive manufacturing (AM), especially laser powder bed fusion (LPBF) technology, has been gradually adopted as an efficient method for fabricating multifunctional structures. By utilizing LPBF, a new integrated particle damper can be produced by deliberately leaving unfused powder inside the structure, named additively manufactured particle damper (AMPD). It has unique merits, such as neither mass nor cost is increased, and no additional space is required [2-3]. However, the damping mechanism and performance of AMPD are still unclear, more investigation is needed.

This research focuses on investigating the damping mechanism and performance of AMPDs with different cavity partitions experimentally and numerically. A series of particle dampers of 316 L stainless steel with different numbers and sizes of unit cells were produced using LPBF. A complex power experimental method was used to test the damping performance of AMPDs at a frequency range of 200-2000 Hz and an acceleration range of 50-200 m/s2 directly. A numerical simulation approach based on the discrete element method (DEM) was developed to investigate the damping mechanism of the AMPDs.

As a result, the numerical results of the proposed simulation model agreed well with experimental data at a frequency of 200 Hz. A consistently larger clearance between the ceiling of the wall and the powder bed was observed in the AMPDs with larger cavity sizes. Furthermore, dividing a larger cavity of AMPD into several smaller cavities emerged as an effective approach to maintaining the damping performance at higher frequencies.

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Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FATIGUE CRACK PROPAGATION BEHAVIOR ANALYSIS OF 15MNTI STEEL BASED ON CYCLIC COHESION MODEL

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ABSTRACT

15MnTi steel is widely used in high load structures such as Bridges, pressure vessels, ships and vehicles due to its excellent mechanical properties. In the course of service, the failure of steel structure is mostly caused by fatigue fracture. In order to investigate the crack growth of 15MnTi steel under fatigue load, the cohesive zone model (CZM) was used to simulate the crack growth. The cohesive zone mode can simulate brittle and plastic fracture behavior by using the function of crack interface opening force and opening displacement to avoid the stress singularity of crack tip. On this basis, a cyclic cohesive zone model was established to study the fatigue crack propagation behavior. This model effectively links damage, tractive force, and cumulative displacement while incorporating the process of fatigue crack growth to accurately simulate material damage evolution under fatigue load. Experimental studies on crack growth in 15MnTi steel at three stress ratios reveal a linear relationship between crack growth rate and stress intensity factor range for different stress ratios. The parameters of Paris formula were calculated using crack growth rate and stress intensity factor range, which provided reference for the selection of model parameters. By utilizing the finite element software Abaqus user element subroutine (UEL) and compiling the cyclic cohesive zone model using Fortran language specifically for 15MnTi steel, simulations were conducted to analyze the evolution of crack tip state under various stress ratios and discuss the corresponding crack growth behavior based on experimental observations. The results demonstrate that the fatigue crack propagation rate varies linearly with both stress ratio range and stress intensity factor range, consistent with experimental findings. The results of the opening and closing evolution of the crack tip are consistent with the law of crack propagation, which indicates that the plastic behavior of the crack tip can be effectively characterized by the cyclic cohesive zone model. Furthermore, parameters obtained from the cyclic cohesive zone model's Paris formula closely match experimental data, thus validating its accuracy and feasibility in simulating fatigue crack propagation behavior.

Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GEOTAICHI: A TAICHI-POWERED HIGH-PERFORMANCE NUMERICAL PACKAGE FOR MODELING MULTISCALE AND MULTIFIELD PROBLEMS IN GEOTECHNICS

Ning Guo[*1], Yihao Shi[1] and Zhongxuan Yang[1]*

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ABSTRACT

This study introduces GeoTaichi, a high-performance numerical package designed for modeling multiscale and multifield problems in geotechnics based on the Taichi parallel programing language. It aims to provide a user-friendly, extensible, and accessible framework that can harness modern computer resources, including multicore CPUs and GPUs. While GeoTaichi is implemented in pure Python, it exhibits scalability and efficiency in solving large-scale problems.

The study primarily focuses on three modules currently available in GeoTaichi: the discrete element method (DEM), material point method (MPM), and the coupled method (MPDEM). The paper outlines the code structures and highlights the most significant features of GeoTaichi. Several benchmark tests are conducted to demonstrate the validity and robustness of the package. Furthermore, the performance of GeoTaichi is compared with similar codes in the field. The DEM simulation results reveal that GeoTaichi exhibits good scaling characteristics when the particle number exceeds 0.3 million on GPU. It is also shown that the DEM module in GeoTaichi offers approximately 70% speedup compared to similar tools utilizing GPU, while reducing memory usage by 350%. Moreover, the coupling scheme MPDEM in GeoTaichi proves to be significantly more efficient than other in-house codes with similar functionalities.

Numerical methods, mathematical modeling and analysis in material science
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RESEARCH ON HYBRID STRESS FINITE ELEMENT METHOD IN MULTIPHASE COMPOSITES AND CAE SOFTWARE DEVELOPMENT

Ran Guo[1], Rui Zhang[1], Wenhai Gai[1] and Yangming Su[1]*

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ABSTRACT

Aiming at the CAE technology in industry, our team, leading by the presenter, has been focusing on hybrid stress finite element method(VCFEM), and developing the core of CAE technology, the new element methods, for more than 20 years under the continuous funding of several National Foundations, and has achieved some results in material damage modeling simulation. The team has made a number of achievements in material damage simulation: a series of new VCFEM elements containing complex microstructures (e.g., inclusions, voids, and cracks, etc.), considering damage evolution, and simulating the whole process of crack initiation and expansion; a micro-meso-macro multiscale method, which realizes cross-scale simulation of damage evolution; a series of high-efficiency and high-precision solid-solid coupling methods; and a series of high-efficiency and high-precision solid-strength coupling methods. A set of CAE software for material damage analysis has been developed, with more than 500,000 lines of code in Fortran, C++ and Python, which realises the damage evolution analysis of real multi-phase materials with millions of microstructures (inclusions, voids or cracks).

Computational mechanics in Canada and China: Current states of shared scientific interests and opportunities for the future cooperation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTATIONAL PHYSICAL MECHANICS: FROM ADVANCED MATERIALS TO HYDROVOLTAIC SYSTEMS

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ABSTRACT

Our understanding of the nature and universal and our ability of creation and production depend on how small we can see (spatial scale), how fast we can capture (temporal scale) and how weak signal we can distinguish (energy scale). When the spatial scale goes down from macroscale to micro-, nano- and pico-meter scale, temporal scale reduces from second to femto- to atto-second, and more importantly, the related energy scale of an externally applied field drops for eighteen orders from joule to atto-joule (1 nN times 1 nm = 6.42 eV), falling into the energy scale of the local fields of matter which consist of electronic structures, charge, molecular orbital and spin states, or well enter the regime of quantum mechanics. Therefore, at nanoscale, matters show distinctly different performances from their bulk materials mainly due to the strong coupling between the local fields of matter and external applied fields, turning common materials such as carbon, even insulators, into functional nanomaterials with exceptional properties we expected for nanoelectronics, spintronics as well as energy conversion devices. Now our experimental ability in spatial, temporal and energy resolutions has experienced revolutionized advance. This revolution opens up a new way for new functional devices and efficient energy conversion technology, but also raises great challenges for computational physical mechanics.

Just as water breeds life, when water meets nanomaterials, the local fields of water molecules, ions, protons and nanomaterials will inevitably be coupled at liquid-solid interfaces, harvesting electricity from water by the novel hydrovoltaic effects we have discovered in the last decade, creating new generation artificial intelligence, leading to intelligent hydrovoltaics for understanding our brain. generating new intelligent characteristics and green energy technology.

In this talk, 1) the rich force-electric-magnetic-optic-thermal coupling functional characteristics and the latest progress of computational physical mechanics will be reviewed; 2) the multi-field coupling effect at the solid-liquid interface of functional materials and water, especially the hydrovoltaic effects, and the recent advances; 3) consider the sustainable development challenge, the basic scientific questions of hydrovoltaic energy, ecology, and intelligence will finally be discussed.

A SYMPLECTIC DEEP AUTOENCODER FOR HAMILTONIAN SYSTEMS

Wei Guo[*1]*

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ABSTRACT

In this talk, we introduce a novel symplectic deep autoencoder for model order reduction (MOR) of simulating parametric Hamiltonian systems with high dimensional state variables. The existing MOR techniques for parametric Hamiltonian systems suffer two limitations. First, the inherent symplectic structure of Hamiltonian systems is not necessarily inherited by the reduced order model. This may lead to instability and blowup of the system energy. Second, due to non-dissipative nature of Hamiltonian systems, the popular global linear subspace solution representation becomes less effective, and it is related to the slow decay of the Kolmogorov n-width of the solution manifold. To overcome the difficulties, we propose a deep autoencoder using HenonNets that can preserve the symplectic structure. HenonNets are constructed by composing a sequence of Henon maps which are parametrized by neural networks. Since a Henon map is symplectic, a HenonNet preserves symplectic structures when used to learn a nonlinear embedding of the solution manifold. Hence, the reduced system is still Hamiltonian, and the system energy and long-term stability is preserved. A collection of numerical tests is presented to verify the effectiveness of the proposed MOR technique.

Uncertainty quantification and reliability analysis in engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RELIABILITY ANALYSIS AND DESIGN OF MULTI-LINE DYNAMICALLY INSTALLED ANCHOR

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ABSTRACT

A novel multi-line dynamically installed anchor was previously proposed by the author to allow for the mooring of multiple floating devices, resulting in a significant reduction in the total number and cost of anchors required for floating wind farms. This study focuses on performing reliability analysis and design for the multi-line dynamically installed anchor, taking into account the spatial variability of soil properties and the uncertainty of loads. To begin, a method is proposed and validated to reduce the number of random variables used in the Karhunen-Loève expansion, aiming to improve computational efficiency while maintaining accuracy. Building upon this, the study combines the random finite element method with the Kriging model and Monte Carlo simulation to investigate the random capacities and probabilistic VHMT failure envelopes of the multi-line dynamically installed anchor in spatially variable soil. A procedure for analyzing the design failure envelope of the multi-line anchor in spatially variable soil is proposed. Finally, the reliability design of the multi-line dynamically installed anchor is conducted and compared with the reliability design of multi-line pile anchors when considering the spatial variability of soil as well as the uncertainty of loads. The results demonstrate that the cost for the multi-line dynamically installed anchor is less obvious than that of multi-line pile anchors. Overall, this study provides valuable insights and methodologies for the practical engineering design of multi-line dynamically installed anchors.

Topology optimization for additively manufactured metamaterials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION FOR MULTI-AXIS ADDITIVE MANUFACTURING

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ABSTRACT

Compared to 3-axis additive manufacturing, multi-axis additive manufacturing has the advantage of reducing self-supporting structures. In 3-axis additive manufacturing, the angle between the structure and the direction of gravity, also known as the overhang angle, is unchangeable. This leads to the necessity of using support materials when the overhang angle is below a certain angle (threshold). However, in multi-axis additive manufacturing, this situation can be addressed by rotating the direction of the printing platform to increase the overhang angle beyond this threshold, eliminating the need for support materials. Therefore, multi-axis additive manufacturing brings new opportunities for the design of self-supporting structures.

This work proposes a self-supporting topology optimization design method for multi-axis additive manufacturing. This method concurrently optimizes both the structural shape and fabrication sequences. Optimized parameters include the material distribution of the structure, printing order, and the rotation angles of the printing platform. The proposed method establishes the overhang constraint using a novel convolution approach, which avoids the commonly observed "dripping effect" in self-supporting designs. Regarding the fabrication sequences, a pseudo-time field is introduced to represent the printing order. The manufacturing process can be divided into multiple steps by partitioning the time field. In each step, the printing platform angle remains constant, and the structure printed in this step is self-supporting. Moving to the next step, the printing platform angle can be optimized and changed, while ensuring that the structure printed in this step remains self-supporting relative to the new printing platform angle. This process is repeated until the printing is completed. For simplicity, we assume a constant fabrication speed, i.e., each step has the same material volume. In addition, this work also addresses the avoidance of collisions between the print head and the already printed structure by introducing a collision constraint. In this constraint, users can define the direction and shape of the print head.

The results obtained through the proposed method not only yield optimized self-supporting structures but also provide an interference-free manufacturing process for multi-axis additive manufacturing. Numerical and printing results will be presented to demonstrate the feasibility of this method.

Buckling analysis and design of thin-walled structures based on novel and intelligent computational methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ISOGEOMETRIC DYNAMIC STABILITY ANALYSIS OF COMPOSITE SHELL STRUCTURES

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ABSTRACT

The load carrying capacity of thin-walled structures is known to be significantly influenced by stability aspects such as buckling. A reliable prediction of buckling phenomena requires a robust and accurate analysis tool and consideration of a number of inherent structural imperfections which often dominate the overall non-linear elastic response. In this contribution, we will study the dynamic buckling problems of composite thin-walled structures in the framework of isogeometric analysis considering geometric imperfections. Our approach exploits the higher order approximation and continuity properties of NURBS modelled shell structures and considers arbitrary openings and cut-outs, as common in industrial applications. We will present a number of challenging shell buckling problems to reveal and assess the reliability and accuracy of the isogeometric analysis approach for geometric imperfect thin-walled composite structures. Besides, different types of dynamic loads and stacking sequences are evaluated and their influence on the dynamic buckling behaviors of the composite shell structures are studied in detail.

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Physics-based data-driven modeling and uncertainty quantification in computational materials science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A DEEP LEARNING APPROACH TO MICROSTRUCTURE-RESOLVED MULTISCALE MODELING, OPTIMIZATION AND UNCERTAINTY QUANTIFICATION

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ABSTRACT

Efficiently modeling material behavior and properties across multiple scales is crucial for designing heterogeneous materials with enhanced properties. However, multiscale modeling by creating a full-scale finite element (FE) discretization of multiscale resolution is often prohibitively expensive. Moreover, employing an FE-squared based multi-level discretization approach introduces errors along element boundaries and is highly dependent on the choice of micro-scale boundary conditions. To address these challenges, we propose a novel deep learning based approach to bridge scales in multiscale mechanics modeling. Our novel U-Net deep learning model, based on a convolutional neural network (CNN), is trained on a small dataset comprising complex microstructures and their corresponding stress tensor fields. By learning the underlying physics from micro-scale simulations, the deep learning model transfers this knowledge to conduct multiscale analysis of macroscopic boundary value problems at micro-scale resolution. Demonstrating a robust ability to generalize, our approach is applied to model various complex materials. We compare the results of our deep learning-based approach with conventional multiscale modeling methods across a range of macro-structure shapes, loadings, and boundary conditions. Additionally, we showcase the versatility of our approach in applications such as uncertainty quantification, multiscale design, and microstructure-resolved multiscale optimization.

Continuum biomechanics of active systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A TRIPHASIC MODEL FOR THROMBUS GROWTH AND FORMATION USING REALISTIC GEOMETRIES

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ABSTRACT

Aortic Dissection (AD) carries a high mortality rate, with approximately 40% of individuals with type B AD living for less than a month. The onset of AD involves a tear in the inner layer (intima) of the aortic wall. This leads to the formation of a secondary blood-filled channel called a false lumen where thrombosis occurs. Given the challenging prognosis of AD, a computational model is presented to understand thrombus formation and growth. Given the complexity of biological systems, we use a macroscopic continuum-mechanical approach based on the Theory of Porous Media.

The model categorizes the aggregate into solid, liquid, and nutrient constituents. The constituents are assumed to be materially incompressible and isothermal, and the whole aggregate is assumed to be fully saturated. Fluid flow in the porous media is described by Darcy's law, and the volume fractions quantify the constituents. Therefore, the regions with thrombus formation are determined using the solid volume fraction. The balance equations consist of coupling terms that represent mass exchange and interactions between phases. These terms are crucial for modelling thrombus formation and growth.

The study introduces equations and numerical examples specific to thrombosis in type B AD. We present the initial studies using 2D geometries. The simulations show that the thrombus grows in the low-velocity regions of the blood. We further study the impact of different parameters on thrombus growth. Thereafter, we extend the triphasic model to 3D geometries to simulate thrombosis and present the model’s usefulness in actual cases. Overall, the proposed model offers a cost-effective approach for numerically simulating thrombosis, providing valuable insights into the understanding and prediction of thrombus development in AD.

Advanced numerical methods for the modeling and optimization of coupled dynamical systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A ROBUST COMPUTATIONAL METHOD FOR COUPLED PROCESSES IN INELASTIC MATERIALS UNDER ACTIVE DAMPING REGIMES

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ABSTRACT

A robust computational method for investigating the thermomechanical response of physically inelastic non-linear systems to dynamic loading was developed. A non-linear dynamic problem of thermo-electromechanics for layered beams was formulated using the Kirchhoff–Love hypotheses. For the case of harmonic loading, a simplified formulation was given based on a single frequency approximation and utilizing the concept of complex moduli to characterize the non-linear cyclic properties of the material. As an example, the forced vibrations and dissipative heating of a roller-supported beam were considered. The developed formalism of thermo-electro-mechanical problem was used for estimating the self-heating caused by the electromechanical losses in piezoactive layers and the mechanical losses in electrically passive metal layer. The heating temperature evolution with time was computed. It was shown that even very small temperature increases due to the dissipation of electromechanical energy over the single vibration cycles may lead to a significant temperature rise for the multi-cycle processes. Following [1-3], the cyclic behaviour of PZT was considered to be a viscoelastic one with relatively small loss moduli. Complex moduli for this material were assumed to be independent of the frequency, temperature, and strain intensity. To avoid dangerous overheating, safe vibration regimes were found. For this purpose, the thermal fatigue life characteristic was introduced. It corresponds to the classical fatigue life, but with the Curie temperature taken as the failure criterion. To prevent overheating, active suppression of the vibration can be used. This was illustrated by numerical examples. The developed method was also successfully used for describing the thermal state under active damping regimes for other thin wall structures with piezoelectric layers for the case of small to moderate inelastic strains in the metal layer.

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Fracture, damage and failure mechanics of cementitious materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING THE QUASI-BRITTLE FRACTURE OF STRUCTURAL MATERIALS USING A MIXED STABILIZED TWO-FIELD FINITE ELEMENT FORMULATION

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ABSTRACT

The fracture process zone (FPZ) is typically characterized as a small region around a crack where non-linear phenomena occur, such as plasticity. In brittle materials, this zone is small and can be safely neglected. However, in quasi-brittle materials, which exhibit a combination of brittle and ductile behavior rather than a clear manifestation of either, the material within the FPZ tends to damage and displays a softening curve after reaching peak load. This behavior is frequently observed in structural materials like concrete and timber, and it can be challenging to model due to its dependence on several factors, including: load type (tension or compression), fiber orientation (particularly relevant for timber), and the presence of a structural size effect.

Traditionally, displacement-based irreducible Finite Element (FE) formulations have been widely used for simulating structural materials like concrete or timber. However, this approach comes with significant drawbacks, such as mesh dependence and convergence problems, when applied to certain phenomena like softening, localization, and fracture. To address these challenges, various techniques have been employed, including extended FE methods, gradient-enhanced models, and phase-field modeling.

In this work, we propose the utilization of a mixed finite element (FE) formulation in which both displacement and strain serve as primary unknowns within the system. To ensure satisfaction of the Ladyzhenskaya–Babuška–Brezzi (LBB) condition, which is associated with saddle point stability in mixed formulations, we employ the Variational Multiscale Method (VMS) to introduce stabilizing terms into the system. Implementation is conducted using FEniCS, an open-source FE software that offers a high-level programming interface written in Python, enabling direct manipulation of the equations' variational form. We validate the implementation by comparing the obtained results with those reported in the literature for a series of simulations involving notched specimens. As failure criteria, we adopt Rankine and Drucker-Prager models, complemented by an exponential softening law that has been modified to capture structural size effects.

The results demonstrate remarkably good performance in terms of both force-displacement curves and stability of the solution field, even when using low-order interpolation elements and irregular meshes. Despite a slight increase in CPU time, the formulation accurately predicts the maximum load, softening curve, and structural size effect in various specimens, exhibiting minimal mesh dependence.

Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

UNSTRUCTURED MESH OPTIMIZATION FOR HYPERSONIC FLOWS ACROSS FLOW REGIMES

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ABSTRACT

The present work discusses the development of High-Altitude Low-Orbit 3D [1,2] (HALO3D), a monolithic software system built to compute aerothermal loads on future hypersonic civilian aircraft. The HALO3D-Navier-Stokes (HALO3D-NS) module uses an edge-based Finite Element (FE) approach for the RANS equations and is capable of accounting for thermo-chemical non-equilibrium, electromagnetic interactions, finite-rate surface chemistry, and weak-ionization. This can be transparently linked to the ablation, rarefied-regime Direct Simulation Monte Carlo (HALO3D-DSMC), and mesh optimization (OptiGrid) modules [3]. At intermediate Knudsen regimes, a hybrid NS-DSMC framework (HALO3D-HYBRID) is used to obtain the flow solution, which is more accurate than a full-NS computation and is faster than a full-DSMC computation. The mesh optimization approach generates optimized meshes that improve solution quality across Reynolds, Mach, and Knudsen regimes. Moreover, a set of mesh optimization cycles for NS takes less time than a single structured mesh computation of similar accuracy. Improved inter-particle collisions and solution quality have also been observed with optimized meshes for both HALO3D-DSMC and HALO3D-HYBRID. OptiGrid functions by equidistributing an error estimate of a set of flow variables throughout the domain, and this is evident in all the flow regimes considered, thus showing that OptiGrid is regime- and solver-independent. The error estimate is constructed from the Hessian of a scalar set of flow variables and electric potential for Magnetohydrodynamic applications. Equidistributing this error estimate dramatically improves the scalars while, interestingly, often reducing mesh size. This presentation showcases benchmark simulations enabled by OptiGrid for complex geometries at different flow conditions, along with plots of the error estimate. The user- and mesh-independent aspects of OptiGrid are also evident across flow regimes through mesh convergence studies that show different initial meshes of any arbitrary quality converging to statistically identical meshes. Such mesh convergence studies go much further than heuristic or sequential refinement approaches and truly eliminate the effects of the mesh on the solution, thus filtering the effects of the flow module. These aspects of OptiGrid illustrate the effectiveness of such an approach in producing “certifiable” flow solutions.

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Finite element techniques for wave simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PARASDG: A PARALLEL–ADAPTIVE SPACETIME SOLVER FOR HYPERBOLIC SYSTEMS

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ABSTRACT

We present ParaSDG, a distributed implementation of an adaptive cSDG (causal Spacetime Discontinuous Galerkin) solver. The cSDG method is a powerful numerical scheme for solving hyperbolic systems of PDEs that features local conservation properties, linear computational complexity, unconditional stability without stabilization, supported by powerful adaptive space-time meshing capabilities. In lieu of synchronous time marching, it constructs unstructured spacetime meshes according to a causality constraint that localizes the solution process to small clusters of spacetime elements called patches. The solution on each patch depends only on adjacent, previously-solved spacetime elements and prescribed initial/boundary data. This structure supports an efficient asynchronous patch-by-patch solution procedure.

We focus in this presentation on ParaSDG's distributed architecture which features a fine-grained, patch-wise parallel structure in lieu of traditional domain decomposition and novel stochastic procedures for dynamic balancing of distributed data storage and computational load. ParaSDG presents a lock-free, task-based architecture in which all processes communicate and execute asynchronously. Solver processes handle the bulk of the computation (spacetime patch construction, localized patch solution, and adaptive meshing) as embarassingly parallel work in process-private memory. Server processes manage a space-like front mesh, the only distributed data set in ParaSDG. Patches represent the basic unit of parallel computation, so there are no domain decompositions. Wrangler processes communicate with t he servers via an MPI layer to isolate the solvers from the latency of accessing the distributed data. In particular, each wrangler extracts and feeds fragments of the front mesh to a paired solver and updates the front mesh with new patch solutions. Wranglers and solvers communicate via lock-free queues in interprocess shared memory for efficient asynchronous execution. Numerical examples demonstrate ParaSDG's adaptive meshing capabilities and scaling performance in problems set in two and three spatial dimensions.

16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics

July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VARIATIONAL FORMULATION OF ELASTODYNAMICS FOR A SPACETIME DISCONTINUOUS GALERKIN METHOD

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ABSTRACT

We present a new spacetime formulation of linear elastodynamics based on Hamilton's Principle of Stationary Action using differential forms and the exterior calculus on manifolds. In previous work, we formulated the same problem using an energy-based, rather than action-based, format to weakly enforce the Equation of Motion and the constitutive relations. This improved formulation supersedes the earlier one. It replaces the purely kinematic independent spacetime fields (displacement, velocity, strain) with mixed kinematic and force-like fields (displacement, linear momentum density, stress). As before, we identify these tensor fields as components of two tensor-valued differential forms in d spatial dimensions: displacement u (a 0-form) and the spacetime momentum flux M (combines linear momentum density and stress into a single spacetime d-form). We formulate the governing equations of motion and constitutive relations in terms of these two forms, their exterior derivatives, and material parameter fields for elastic response and material density. The spacetime exterior derivatives include jump parts to support our intended implementation on spacetime broken Sobolev spaces. After formulating a Lagrangian Functional of (u, du, M and dM) we apply Hamilton's Principle and Stokes Theorem to obtain a weak problem statement that is simpler than the previous one. Expressing all jump terms with respect to Riemann solutions yields unconditionally stable finite element formulations. We describe an implementation in ParaSDG, a distributed discontinuous Galerkin solver with adaptive spacetime meshing capabilities in up to E^3 x R, and present numerical results to demonstrate the new formulation's accuracy, efficiency and convergence properties.

PSE (Problem Solving Environment)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT OF A LAND USE CLASSIFICATION MODEL BASED ON SEMANTIC SEGMENTATION USING AERIAL PHOTOGRAPHS AND ITS APPLICATION TO TSUNAMI SIMULATION

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ABSTRACT

This paper presents the development of a land use classification model based on semantic segmentation using aerial photographs. The land use data is an important part of geospatial information and can be used in a wide variety of urban development planning and disaster prevention measures. However, these data have been of limited use to date due to their low update frequency and the difficulty of obtaining high resolution data. In previous studies [1], several single-category segmentation models have been built mainly for roads and buildings, creating a limited data set.

The purpose of this study is to create a high-resolution, multi-category land use data set using aerial photographs and the deep learning method. We focused on the method of data expansion, batch size, and CNN hierarchy to obtain quantitative knowledge of the effect of these parameters on the classification results. For the deep learning model for semantic segmentation, the PSPNet (Pyramid Scene Parsing Network) [2] is employed. In order to examine the validity of multiple classification models developed with different parameters, aerial photographs of the target area were applied to this model. Furthermore, we applied the segmentation results to a two-dimensional tsunami run-up simulation and verified their contribution to improving the performance of the simulation.

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Complex fluid flows in engineering: Modeling, simulation, and optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SIMULATION AND OPTIMIZATION OF PHOTOVOLTAIC PANEL ARRAY CONFIGURATIONS IN WIND FLOW

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ABSTRACT

Among the renewable energy solutions of today, solar - more specifically photovoltaic (PV) - power plants are seen as key actors of the energy transition in Europe, and are taking on new designs and functions, seeking more adaptability and efficiency. However, PV power plants still face the major risk of strong winds often leading to breakage, hindering the efforts of green energy development. The aerodynamic loading of PV panels in wind flow has become an important research topic to quantify breakage risk and limits, but such approaches in the literature have been limited so far to panel spacing and simple tilt configurations. We introduce here a novel approach combining high-fidelity numerical simulations of large scale PV fields subjected to a turbulent atmospheric boundary layer wind flow, and a Deep Reinforcement Learning (DRL) algorithm trained to optimize the individual tilts for the purpose of maintaining safe aerodynamic efforts. An efficient and flexible computational pipeline has been developed, in which the mesh is adapted anisotropically around the fluid-solid interface using a metric map built after simulation-dependent parameters based on the boundary layer theory. The wind flow is computed with an in-house variational multiscale (VMS) stabilized finite element solver. The latter can be applied efficiently to high Reynolds number flows (since the built-in small-scale component of the solution operates as an implicit large eddy simulation) and supports elements of aspect ratio up to the order of 1000:1, which is key to solve the numerically complex strongly anisotropic wind motion generated by the extremely thin build of the panels. Finally, DRL optimization is achieved with the in-house single-step PBO algorithm, that interacts once per episode with the environment to learn the mapping from a given initial state to the optimal action, and uses heuristics from the CMA-ES evolution strategy to exploit the anisotropy of the cost function in the descent direction. The main sub-processes of PV field simulations are seamlessly integrated within a single agent-environment workflow. This includes the geometric computational domain creation from an array of panel tilts, the mesh adaptation algorithm, CFD simulations, and reward computation. We will discuss results obtained for 2d and 3d arrangements of 6 full-scale panels mounted on stands, whose individual tilts are optimized under various reward functions and using different turbulence models. Each optimal configuration is non-intuitive and reward-specific, and will be shown to perform better than the classic tilt configurations found in the literature.

Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A STOCHASTIC MULTISCALE MODELING METHOD BASED ON THE INTERACTION BASED DEEP MATERIAL NETWORKS FOR HIGHLY DISSIPATIVE STRUCTURES ADDITIVELY MANUFACTURED WITH SELECTIVE LASER SINTERING

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ABSTRACT

Additive manufacturing techniques offer new opportunities to produce high quality structures with enhanced performances. In particular, selective laser sintering was recently used to fabricate lattice structures for high energy absorption applications. The printed parts seem homogeneous at surface. However, upon close examination, micro-porosity appears and has significant influence on the structural behavior. This created porosity is non-uniformly distributed across the structure, making classical multiscale approaches, such as FE2, not adequate to address this problem due their intensive computational burden.

In this study, we present a stochastic multiscale modeling method to address structures with non-uniform distribution of porosity at micro-scale. The method is based on the interaction-based deep material network (IB-DMN). The IB-DMN aims to determine an accurate low-dimensionality representation of the microstructure topology, which will substitute the microscopic FE model during the multiscale analysis. This will considerably alleviate the computational cost. The IB-DMN is a network composed by nodes linked through interaction mechanisms, both of them characterized by attributes. It is able to replace microscopic FE problem when it is able to accurately replicate its effective behavior for any arbitrary loading cases. This is achieved through a pre-processing step during which the network attributes are tuned to align IB-DMN predictions with FE results. Once trained, the IB-DMN is employed as a surrogate in the multiscale analysis.

We extended the method into two main directions. First, the material used during the printing process exhibit a coupled viscoelastic-viscoplastic (VE-VP) behavior. We included viscous effects in addition to history dependency to account for this behavior, which were not previously studied. Secondly, we developed the porosity guided IB-DMN (PgIB-DMN) to effectively address the variable porosity ratios across the structure without training. This new method consists on the construction of limited number of base IB-DMNs with known porosity ratios. Afterwards, the behavior of any new microstructure is computed by combining the responses of the base DMNs.

The IB-DMN was trained using only elastic and elastoplastic data. Its generalization performances were investigated for new VE-VP porous materials under different loading conditions and across various strain rates. The performances were extensively compared to FE simulations and mean filed homogenization. Overall, the reduced model demonstrated remarkable extrapolation capabilities and speedup. The PgIB-DMN allows to accurately predict the behaviors of new microstructures without requiring any additional training. Additionally, it permits to effectively carry out stochastic multiscale analysis accounting for the continuously variable porosity.

A GRAPH NEURAL NETWORK TECHNIQUE FOR SHAPE OPTIMIZATION: APPLICATION TO MULTI-OBJECTIVE FLUID-ACOUSTICS OPTIMIZATION

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ABSTRACT

Aero/hydroacoustic noise is a major concern in the design of marine propellers, and wind turbine blades that can be minimized through shape optimization. To this end, we propose a novel data-driven approach based on the Finite-Element Inspired Graph Neural Network (ϕ-GNN) proposed by [1] for shape optimization applications. GNNs demonstrate effectiveness in handling arbitrary unstructured meshes without requiring model modifications. Our study focuses on employing ϕ-GNN for the reduced-order modeling of the Navier-Stokes equations to alleviate the computational costs inherent in shape optimization. Of particular interest is to predict incompressible flow fields for varying shapes in 2D high-Reynolds number flows. The proposed model can efficiently predict the quantities of interest for various shapes based on the provided mesh and physical parameters.

The proposed technique relies on an Encode-Process-Decode structure. Grid vertices in a computational fluid dynamic domain are treated as nodes and used as inputs to the graph neural network. These nodes are initialized with physical parameters, including angle of attack and Reynolds number, to pass messages on a mesh graph. They learn a mapping between spatial positions and the target data generated by the full-order Navier-Stokes computations. We demonstrate the effectiveness of the network by predicting the flow field around a wide range of airfoils to obtain the airfoil broadband self-noise resulting from the interaction of a turbulent boundary layer with a sharp trailing edge. Far-field noise is evaluated using Amiet's theory [2] to calculate the wall pressure spectrum based on the boundary layer parameters. We extract the boundary layer parameters from the network, and the results are compared with the full-order computations. The findings indicate that the online flow field around an airfoil can be predicted in seconds, which is hundreds of times faster compared with the full-order results. Finally, we integrate the network with a multi-objective optimization algorithm to minimize the overall sound pressure level while ensuring favorable integrated quantities of interest.

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Computational methods for wind energy
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

WIND TURBINE DAMAGE EQUIVALENT LOAD ASSESSMENT USING GAUSSIAN PROCESS REGRESSION COMBINING MEASUREMENT AND SYNTHETIC DATA

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ABSTRACT

Assessing the structural health of operational wind turbines is crucial, given their exposure to harsh environments and the resultant impact on longevity and performance. However, this is hindered by the lack of data in commercial machines and accurate models based on manufacturers' proprietary design data. To overcome these challenges, an innovative approach to evaluate and predict loads in wind turbines using Gaussian Process Regression (GPR) is proposed. The study introduces a method that blends aero-servo-elastic simulations of publicly available wind turbine models and real-world data from Supervisory Control and Data Acquisition (SCADA) systems to create a hybrid database. By incorporating both simulated and real-world data, we aim to overcome the limitations of each data type and enhance the model's predictive accuracy. Then a GPR model is trained on the hybrid data. The GPR model validation involves an extensive analysis of a year's worth of SCADA data from an operational wind turbine. The results demonstrate the GPR model's ability to interpret and predict turbine performance, confirming its potential as a reliable tool in the structural health monitoring and load prediction of wind turbines. The accuracy of the model is further highlighted through its ability to predict turbine loads under various wind speeds, which is critical for ensuring the longevity and efficiency of wind turbines. This research discusses the broader applications of this approach in the field of asset reliability and health management. The methodology can be adapted to address the challenges associated with limited data availability in commercial wind turbines, thereby contributing to the overall advancement of predictive maintenance strategies in renewable energy systems.

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Data-driven approaches for solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LATTICEGRAPHNET: A TWO-SCALE GRAPH NEURAL OPERATOR FOR SIMULATING LATTICES AND STRUCTURES

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ABSTRACT

This study introduces a two-scale Graph Neural Network (GNN), namely, LatticeGraphNet (LGN), designed as a surrogate model for replacing costly nonlinear finite-element simulations of three-dimensional latticed parts and structures. The LGN architecture is based on MeshGraphNet [1] but with two networks: LGN-i, which learns the reduced dynamics of lattices, and LGN-ii, which learns the mapping from the reduced representation onto the three-dimensional tetrahedral mesh. LGN can predict deformation for arbitrary input lattices.

Our pipeline is trained on a set of high-fidelity nonlinear Neo-Hookean finite-element simulations with large deformation, buckling, and self-contact considerations and evaluated by studying the compressive response of lattices on unseen geometries. Every simulation step deforms the tetrahedral mesh at a rate of 20 mm/s for a total of 0.315s using 15 implicit time steps. However, the complexity of FEA simulations results in a long runtime, on the order of 48 hours to 10 days per model, depending on the mesh size, topological characteristics, and nonlinearities due to buckling and self-contact, therefore the need for speed up using machine learning.

We find that our approach provides reasonable responses until 25\% compressive strain and can predict nonlinear behavior such as buckling. Homogenization of the LGN outputs showed similar force correlations with FEA simulations but contained inaccuracies. LGN significantly reduces inference time while maintaining high accuracy for unseen simulations, hence establishing the use of GNOs as efficient surrogate models for evaluating mechanical responses of lattices and structures. To our knowledge, this is the first study that tackles the three-dimensional response of lattices with nonlinearity and buckling considerations.

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Recent advances in meshfree and particle methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NEW SPAR TYPE FLOATING WIND POWER PLANT BEHAVIOR SIMULATION FOR REDUCTION OF MOTION BY SPH METHOD

Seiya Hagihara[*1], Rikuto Ideta[1], Yuhi Uchino[1], Satoyuki Tanaka[2], Shinya Taketomi[1] and Yuichi Tadano[1]*

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ABSTRACT

It is important to stabilize behaviors for the efficiency of the floating wind power plants. And it is necessary to consider safety in the case of a design for the floating wind power plant about the natural disasters such as tsunamis. To predict behaviors of floating wind power plants in the ocean are very important for the safety and the ability of efficiency for power generation by numerical simulations. The particle methods which are the smoothed particle hydrodynamics (SPH) method [1] and the moving particle semi-implicit (MPS) method [2] are recently applied to fluid dynamics analyses for predictions for behaviors of structures under natural disasters such as Tsunami.

The SPH method including the artificial viscosity coefficient and the artificial density diffusion coefficient are proposed by M.Antuono et al.[3] and D.Molteni et al.[4] that is the δ-SPH method. The numerical correction terms are added to the momentum conservation equation and mass conservation equation in the delta-SPH method respectively. The 3-dimensional delta-SPH method analyses are applied to calculate the behaviour of the conventional and the new spar type wind power plant models. The new spar type has the plate for the reduction of motion. The calculated results are compared with each other.

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High order methods for time-dependent problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HIGH-ORDER METHODS FOR HYPERBOLIC SYSTEMS WITH LOCAL EVOLUTION

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ABSTRACT

For challenging problems in wave theory, it is easy to show that high-order/high-resolution methods are far more efficient than their low order counterparts in terms of degrees-of-freedom required to achieve an acceptable accuracy. However, considering for example standard discontinuous Galerkin discretization schemes, the cost of time-stepping grows rapidly with order, due to the artificial stiffness induced by one-sided differentiation at element boundaries. In this work we conisder methods which circumvent this issue by employing staggered meshes. In particular we will consider methods based on Hermite interpolation as well as staggered DG schemes employing more standard polynomial bases. In both cases we will prove that the degrees-of-freedom in each element can be evolved independently with comparable orders of accuracy in both space and time and with time steps limited only by domain-of-dependence constraints. We will also discuss methods for applying boundary conditions for the staggered schemes. Experiments on multicore and GPU-based architectures will be presented.

Multiphysics and data-driven modeling for cardiovascular biomedicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING LEFT VENTRICULAR ELECTROMECHANICS IN PATIENTS WITH HYPERTROPHIC OBSTRUCTIVE CARDIOMYOPATHY

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ABSTRACT

Hypertrophic obstructive cardiomyopathy (HOCM) is an inherited cardiac disease where the left ventricle (LV) myocardium thickens abnormally around the basal plane, dynamically obstructing aortic blood flow. Untreated HOCM often results in abnormal LV outflow tract pressure gradient and is associated with an increased risk of heart failure and sudden cardiac death. HOCM patients with symptoms refractory to medical management are treated with a surgically performed septal myectomy or a transcatheter-based alcohol septal ablation. While myectomy is the current gold standard, where a surgeon resects the excess myocardium using an open-heart procedure, alcohol ablation involves injecting alcohol at the hypertrophied septum, leading to a permanent scar and restricted motion alleviating obstruction [1].

Both procedures rely heavily on the operator's experience and lack objectivity in predicting their effectiveness to relieve obstruction without causing complications, including perforated septum, heart block, repeat interventions, and arrhythmia. Image-based computational modeling offers a non-invasive platform to perform virtual treatments and evaluate the outcomes of each procedure before intervening on the patient. However, modeling of myectomy and ablation is a challenging task that should account for multiphysics interactions, including electromechanics and blood flow, if the goal is to predict the relief of obstruction. Moreover, both procedures alter the myocardium's structure and function. This underscores the need for a patient-specific modeling framework to develop personalized treatment plans.

As a precursor to the multiphysics model of HOCM, we present a computational workflow to simulate ventricular electromechanics in HOCM patients using time-dependent computed tomographic (CT) images. Our workflow employs a novel inverse finite element analysis (iFEA) framework to estimate passive myocardial material parameters from dynamic CT data, while using state-of-the-art structurally-based constitutive models, accounting for myofiber disarray, and applying physiological boundary conditions [2]. We introduce a novel coupling algorithm between the 3D model and a lumped parameter network (LPN)-based model of the circulatory system, to perform closed-loop multiscale modeling of myocardial mechanics under physiologically relevant loads [3]. We also introduce a novel tuning framework to personalize the multiscale model to clinical measurements and image-based volumes and displacements, and apply the framework to a healthy subject and 3 HOCM patients. Finally, we will discuss our strategy to couple the personalized electromechanics modeling framework with a 3D blood flow model that is instrumental to performing virtual surgery simulations of myectomy and ablation.

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Numerical modelling of composite materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING CONSIDERATIONS IN THE SIMULATION OF SELF-HEALING FIBER REINFORCED POLYMER COMPOSITES

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ABSTRACT

The hierarchical architecture of fiber-reinforced composites (FRC) enables the design of lightweight materials with outstanding mechanical properties. This structure, however, makes FRC uniquely susceptible to interlaminar fracture (i.e., delamination). Recent research has shown that delamination damage can be reversed by Introducing a tough thermoplastic healing agent between individual reinforcing layers, thereby endowing FRC materials with a highly attractive self-healing ability [1-3]. Nevertheless, the effect of softer thermoplastic inclusions on other mechanical properties (e.g., shear), have not been fully explored.

In this presentation, we discuss a computational approach for assessing the mechanical response of glass-fiber composites containing a 3D printed poly(ethylene-co-methacrylic acid) (EMAA) thermoplastic healing agent. We employ 3D finite element models to investigate the impact of EMAA inclusions in a 3-point flexure (i.e., short beam shear) test and validate the numerical model with experimental data. The study emphasizes the impact of different assumptions, including material constitutive models and boundary conditions, on model fidelity and provides guidelines on computationally efficient and accurate modeling of FRC materials with interlaminar inclusions. This work contributes a reliable framework for the computational exploration of material design and illuminates research gaps in the simulation of self-healing composite materials [4].

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FAILURE ANALYSIS IN FLEXOELECTRIC CONTACT MECHANICS

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ABSTRACT

In classical continuum mechanics, maximum principal stresses usually occur directly on the surfaces. However, the equivalent or von Mises stress which is a combination of stress tensor components has its peak value inside the bodies beneath the surfaces. This character is famous in Hertzian contact mechanics, where the maximum von Mises stresses appear beneath the contact surfaces, thus contradicting a common appearance of failures in surface fatigue. In this type of failure, pitting initiates from the surface contacts and rapidly proceeds to failure by spalling. To explain this discrepancy, it has been shown that couple-stresses can cause the critical stress to reach its maximum on the surface [1]. This suggest that flexoelectric effects can have a more significant impact on the mechanical behavior of dielectric bodies especially in contact at micro/nano and macro scales. In particular, the state of deformation and stresses in the vicinity of the contacting area deviates remarkably from what is predicted by Hertzian contact theory [2,3].

In the present work, by using couple stress based flexoelectric theory [2,3], we investigate the distribution of an equivalent von-Mises stress near the contacting area of isotropic flexoelectric bodies. Since analytical solutions for this size-dependent contact problem are not available, we have developed a boundary element formulation to calculate the displacements, rotations, force-stresses, and couple-stresses for two-dimensional isotropic flexoelectric contact problems. The numerical results of this non-linear coupled problem model show interesting characters, which are different from those in classical theory. The significance of flexoelectricity in contact mechanics becomes evident through this study, offering an explanation for numerous unexplained phenomena in the field of tribology.

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Advances in material model calibration for computational solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CALIBRATING CONSTITUTIVE MODELS WITH FULL-FIELD DATA VIA PHYSICS INFORMED NEURAL NETWORKS

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ABSTRACT

The Virtual Fields Method (VFM) and Finite Element Model Updating (FEMU), among other inverse problem methodologies, have shown success in calibrating constitutive model parameterizations for various nonlinear material models. However, VFM faces difficulties when only ingesting full-field surface data for specimens where plane-stress assumptions break down, and FEMU remains challenging when calibrating complex models where computational inefficiencies of the inverse problem are intractable. In this work, we use emerging physics-informed machine learning techniques rather than the aforementioned traditional approaches to calibrate constitutive models in large deformation scenarios using full-field experimental data. Physics-informed neural networks (PINNs) can utilize measured data for model calibration while approximately maintaining the known physical laws of the system. PINNs as a computational tool are meshless, with collocation points that are unconnected, meaning there is no need for interpolation strategies between the full-field measurement grid and the computational grid. In an inverse problem, the unknown material parameters are added to the solution basis like VFM. Rather than shape functions, the solution basis in the case of PINNs are the weights and biases of the neural network. Classical PINNs typically work in terms of the strong form of the governing equations and penalize boundary conditions (BCs) in a weak sense. This approach can make imposing the numerous traction-free boundary conditions in a solid mechanics boundary value problem difficult and furthermore it can have large effects on the solution displacement field by having errors in the displacement BC. Also working in the strong form requires enough smoothness in the activation functions and a fine enough sampling of collocation points to accurately resolve the second derivatives appearing in the governing equations of motion. Our method utilizes a combination of an energy formulation and the principle of virtual work with displacement BCs enforced exactly. In this way we have reduced the smoothness requirements and removed several of the objectives from the loss function involving BCs. Traction free BCs are also satisfied by construction. We formulate a loss function with standard error metrics along with a physics-informed term to minimize the error between observed and predicted data while persevering the balance of momentum approximately. This approach is demonstrated using synthetic data, generated from FEM simulations, representative of full-field experimental data for exemplar problems of materials undergoing large heterogenous deformation to calibrate several hyperelastic constitutive models. We will also present preliminary results utilizing digital image correlation experimental data on simple experimental specimen geometries.

Numerical methods, mathematical modeling and analysis in material science
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

OPTIMIZING THE IDENTIFICATION OF TRANSVERSAL COMPRESSION BEHAVIOR OF A HIGH-STRENGTH SYNTHETIC FIBER USING ADVANCED MACHINE LEARNING ALGORITHMS

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[2]Université Paris-Saclay, ENS Paris-Saclay, CNRS, Laboratoire de Mécanique Paris-Saclay
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ABSTRACT

High-strength synthetic fibers are extensively utilized in ballistic protection. However, accurately determining their mechanical properties through experimentation poses significant challenges due to their small cross-sectional sizes, ranging from 1 to 100 µm. Achieving micro-level accuracy demands substantial equipment and specialized human resources. The presented research aims to optimize the identification of the nonlinear transverse compression behavior of any synthetic fiber. Within this study, over 200,000 data points generated from a finite element model validated through rare experimental data on Kevlar KM2 fibers with a circular cross-section radius of 12 µm, achieving large deformations of up to 18%, were analyzed using advanced AI algorithms. Five algorithms—Elastic Net, Bayesian Ridge, Neural Network, Gradient Boosting, and Random Forest—were employed to identify the optimal AI model based on criteria including minimal training data requirements, ease of accessibility, and the ability to swiftly predict any existing fiber type in reality. The analytical results reveal intriguing findings. The optimized AI models identified in this study do not require data on fiber diameter and Poisson's ratio to generate accurate predictive models. However, the initial elastic modulus and loading history are indispensable for any AI algorithm.

Recent advances in discretization techniques for coupled problems in incompressible fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A SECOND-ORDER UNCONDITIONALLY STABLE BOUND-PRESERVING SCHEME FOR THE QUASI-INCOMPRESSIBLE CAHN-HILLAIRD-DARCY EQUATIONS

Yali Gao[1], Daozhi Han[*2] and Xiaoming Wang[3]*

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[2]State University of New York at Buffalo
[3]Missouri University of Science and Technology

ABSTRACT

In this talk we introduce a quasi-incompressible Cahn-Hilliard-Darcy model for two-phase flows in porous media or Hele-Shaw cell. We then present a second-order accurate, unconditionally stable, mass-conservative and bound-preserving numerical method for solving the model.

Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE MODELING OF CRYSTAL PLASTICITY: ABAQUS FE2 MODEL AND ITS SURROGATE FE-RNN MODEL

Fengbo Han[*1], Kapil Krishnan[1], Jide Oyebanji[1] and Zhongwei Guan[1]*

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ABSTRACT

This study presents a novel multiscale approach to modeling large-strain plastic deformation in polycrystalline materials, utilizing both a two-scale finite element (FE2) method and its surrogate model based on a recurrent neural network (RNN). The FE2 model integrates a full-field crystal plasticity FE model at the mesoscale within a macroscopic FE model, employing the ABAQUS/Standard implicit FE solver for both scales. In this approach, the homogenized stress response from the mesoscale crystal plasticity model informs the integration points of the macroscopic model at each increment. The effectiveness of the FE2 model was validated through a one-element tension test on polycrystalline aluminum, focusing on stress-strain response and texture evolution. Additionally, compression and shear tests on high-resolution representative volume elements were conducted to observe microstructural morphology evolution under deformation. Although the FE2 model demonstrated accuracy, it was found to be computationally intensive. To address this challenge, a faster multiscale model was developed using an RNN as a surrogate for the mesoscale crystal plasticity model, integrated within the ABAQUS/Standard implicit FE solver. The RNN model was trained on a comprehensive dataset derived from single crystal deformation simulations, covering a broad spectrum of grain orientations and strain paths, thus ensuring robustness and adaptability. This multiscale FE-RNN model was then utilized to simulate complex material deformations, achieving efficient and accurate predictions of material behavior under various loading conditions. Comparative analysis with the Abaqus FE2 model confirmed the surrogate model's accuracy and efficiency. This research introduces a powerful multiscale tool for the efficient and precise simulation of polycrystalline materials, offering significant potential for engineering applications.

Current trends in phase-field modeling and computations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CRACK PHASE-FIELD ENHANCED FINITE COVER METHOD REALIZING DIFFUSIVE-DISCRETE CRACK TRANSITION

Jike Han[*1], Yuichi Shintaku[2], Shuji Moriguchi[1] and Kenjiro Terada[1]*

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ABSTRACT

Fracture is one of the most crucial failure mechanisms in engineering fields. As well as the theoretical and experimental developments to understand the failure mechanisms, numerical simulation methodologies have been studied along with the development of computer hardware. In this trend, the crack phase-field model has been receiving significant attention due to its ability to predict arbitrary crack initiation, propagation, and bifurcation phenomena. However, the original theory of the crack phase-field model describes discontinuous crack propagation but eventually behaves the same as a continuum damage model due to the regularization of the discrete crack surfaces to be the diffusive ones. Accordingly, the crack phase-field model suffers from mesh distortion issues and divergence of Newton-Raphson computations. Also, the independent movements of multiple portions divided by crack are unable to be traced.

In this study, we present a transition scheme [1,2,3] from diffusive to discrete crack topologies. The crack transition scheme can trace an actual crack path as closely as possible and stably update its explicit crack surfaces even in a large deformation regime, including plastic deformation. In the proposed scheme, the crack initiation, propagation, and bifurcation are determined from an energy minimization problem with respect to the displacement field and the crack phase-field, while the predicted path represented by a diffuse crack topology is replaced by a discrete one by introducing the finite cover approximation. Since the discontinuity of the displacement field is introduced, the entire braking process and the subsequent independent motions of multiple portions can be captured by one single numerical setup. We present several numerical examples of brittle, dynamic, and ductile fractures to show the stable update from diffusive to discrete crack topologies within the finite strain framework.

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Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREDICTION OF MICRO-SCALE MECHANICAL RESPONSES OF CEMENT PASTE USING SCALE-LINKING MATERIAL PARAMETERS CALIBRATED FROM MACRO-SCALE BEHAVIORS

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ABSTRACT

Determining the mechanical behavior of cement paste at the micro-scale by experiment is difficult due to the uncertainties inherent in cementitious materials. Simulations can be used to complement time-consuming experiments and help accelerate the development of new materials and the performance evaluation of existing materials. The evaluation of micro-scale mechanical responses using simulations is also challenging. However, by synergistically combining experiments and simulations, virtual experiments can be performed on realistic microstructures with accurately identified input material parameters. In this study, a multi-scale framework similar to that used in Ref. [1] is used to simulate micro-scale mechanical responses from material parameters calibrated from macro-scale analysis.

The macro-scale cement paste microstructures are obtained from synchrotron micro-CT measurements and the nanoindentation experiment is performed considering an indentation volume comparable to a voxel volume for macro-scale microstructures. The in-situ macro-scale tensile splitting test with micro-CT is used to calibrate the phase-field fracture model implemented based on Ref. [2]. The calibrated macro-scale model is used to determine the input material parameters at the micro-scale through a scale-linking process using the relationship between the nanoindentation property and the characteristic from micro-CT images, i.e., the linear attenuation coefficient. The multi-scale framework for evaluating micro-scale responses calibrated from macro-scale behaviors is demonstrated by conducting micro-scale virtual experiments such as direct tension and splitting tensile tests, which confirmed the validity of the framework.

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Emerging frontiers and methods in digital manufacturing: Modeling, simulation, and beyond
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPARATIVE EVALUATION OF 3D-PRINTED AUXETIC TITANIUM STENTS: A THREE-POINT BENDING TEST AND FINITE ELEMENT SIMULATION STUDY

Rahul Vellaparambil[1], Woo-Suck Han[1], Pierluigi Di Giovanni[2] and Stéphane Avril[1]*

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ABSTRACT

Conventional stent designs, plagued by limited flexibility, often fail to accommodate the intricate geometries and tortuous paths of endovascular arteries. Auxetic stents, characterized by a unique negative Poisson's ratio, promise enhanced flexibility, offering a promising solution for endovascular applications1. However, the intricate geometries of auxetic stents present a significant challenge for conventional manufacturing techniques.

This study bridges the gap between simulation and reality, evaluating the bending performance of auxetic stents fabricated using 3D printing technology. Employing the Direct Metal Laser Sintering (DMLS) process, we successfully 3D-printed titanium alloy stent prototypes based on auxetic stent designs1 previously investigated. These prototypes were then subjected to rigorous three-point bending tests as per ASTM standards, providing valuable experimental data.

To complement the experimental findings, we developed a comprehensive finite element (FE) model, capable of accurately predicting the bending behavior of both auxetic and conventional stents. The FE model, validated against the experimental data, demonstrated satisfactory accuracy in capturing the bending flexibility of the fabricated stents. Our findings demonstrate the immense potential of 3D printing technologies in fabricating auxetic stents, offering a paradigm shift in endovascular applications. The ability to control intricate stent geometry using 3D printing enables the tailoring of stent design to match the unique anatomies of individual patients. While this study provides a promising foundation for the clinical translation of auxetic stents, further research is warranted to optimize current stent design limitations with 3D printing technologies and incorporate advanced post-processing techniques. By addressing these challenges, we can enhance the reliability and reproducibility of 3D-printed auxetic stents, paving the way for their widespread adoption in endovascular procedures.

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Computational and analytical advances in nonlocal modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ASYMPTOTICALLY COMPATIBLE SCHEME FOR NONLOCAL SADDLE POINT PROBLEMS

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ABSTRACT

In this talk, we present an abstract framework for studying asymptotically compatible schemes for parameterized saddle point problems. This framework is then applied to the study of robust numerical discretization for several nonlocal problems, including nonlocal Poisson's problem, nonlocal Stokes equation, and nonlocal biharmonic problems.

Advanced numerical techniques for fluid flow in porous media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL INVESTIGATION OF THE IMPACT OF NATURAL FRACTURES ON THE PRODUCTIVITY OF PARENT AND CHILD WELLS CONSIDERING FRAC HITS

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ABSTRACT

Abstract: A multi-scale quadruple-medium productivity model for shale gas reservoirs is developed, taking into account gas multiple micro-flow regimes, adsorption effects, and stress sensitivity. This model is based on the principles of poroelasticity and fluid-solid coupling. Subsequently, the model is solved using COMSOL to analyze how the characteristics of natural fractures-such as length, aperture, density, roughness, and dominant orientation-affect the variation in productivity of parent and child wells under frac hits conditions. The simulation results indicate that the production rate of the parent well with frac hits initially experiences a temporary increase followed by a decline, surpassing scenarios without frac hits. In the early stage of child well production, due to frac hits, its rate is lower than the production rate of the parent well. The length, density, and aperture of natural fractures exhibit a positive correlation with the degree of interference, while the dip and roughness of natural fractures show a negative correlation. The impact of natural fracture characteristics on the degree of interwell interference is ranked as density > length > dip > opening > roughness. Among these factors, the impact of natural fracture roughness on production is minimal. When the roughness coefficient changes by 20%, the change rate of production in the parent and child well is only 0.003%, which can be considered negligible. The research findings can guide the prediction of shale gas productivity and the dynamic adjustment of production parameters.

Keywords: shale gas, horizontal wells, frac hits, natural fractures, productivity simulation

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RBF INTERPOLATION METHOD WITH AN ADAPTIVE SHAPE PARAMETER AND A POSTERIORI ERROR ESTIMATION USING SUPERVISED LEARNING

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ABSTRACT

The integration of machine learning methods within PDE numerical solvers to speed-up computation, to account for more detailed descriptions of systems or to improve the quality of the numerical solution has become a common practice. However, often the machine learning models considered are static in nature, they consist of a offline training phase, and once trained are deployed and remain static. This, in turn, places an extreme importance on the correct design of the training set and training procedure, and leads to models which might not be robust (e.g.: when unseen inputs are far away from the training set). In this work, we present a hybrid computation framework in which the machine learning model continuously learns during run-time. In particular, using a novel procedure akin to a posteriori limiting, we obtain a more robust solver by switching between a data-driven method, and a gold standard procedure (which is used to generate the original training data), which in turn will be used to re-train the neural network.

To demonstrate the performance of this framework, we extend our previous work on selecting optimal parameters for radial basis functions approximations. Namely, the choice of the shape parameter highly effects the behaviour of radial basis function (RBF) approximations, as it needs to be selected to balance between ill-condition of the interpolation matrix and high accuracy. Previously, we demonstrate how to use neural networks to determine the shape parameters in RBFs using an unsupervised learning strategy. In this new work, by using error estimators on the network's prediction, we can switch between the data-driven method, and an optimization procedure that can then be used to re-train the neural network.

INTELLIGENT OPTIMIZATION DESIGN FOR VARIABLE-STIFFNESS STRUCTURES

Peng Hao[*1]*

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ABSTRACT

Advanced variable-stiffness thin-walled structures with curvilinearly stiffened paths and curved fiber paths as the main features have attracted significant attention. However, the addition of a large number of control parameters also leads to a rapid increase in the dimension of design variables. This paper proposes an intelligent optimization design method for lightweight variable-stiffness structures based on deep learning technology. The basic idea of this method is to use various convolutional neural networks to identify and extract the complex variable-stiffness structure features, and establish an implicit mapping relationship between the structure layout image and the structure performance. Further, the structural layout image is directly used for modeling the Gaussian process and finding the optimization in combination with the surrogate optimization framework, thus forming a driving force for the optimization process. Compared with traditional methods, both the accuracy of the optimization model and the efficiency of optimization are greatly improved, and the efficient solution of variable-stiffness structure layout design problems with dynamic changes in the number of design variables is realized.

Recent advances on interfaces dynamics modeling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN MODELING OF ALZHEIMER'S DISEASE

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ABSTRACT

With over 5 million individuals affected in the US, Alzheimer`s disease (AD) has become a pressing concern. Personalized treatment plans for AD patients offer a promising new avenue for managing this disease but require novel approaches for analyzing the increasing amount of electronic brain data available. In this talk, we will introduce a mathematical modeling approach for describing the progression of AD clinical biomarkers and incorporating patient data to enable personalized prediction and optimal treatment. Specifically, we will validate this mathematical model on a multi-institutional dataset of AD biomarkers to provide personalized predictions for AD patients.

Advanced materials and smart structures: Modeling, simulation and testing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL EVALUATION OF EFFECTIVE ELASTIC PROPERTIES OF COMPOSITES WITH ROTATIONALLY SYMMETRIC PARTICLES BY A SURROGATE MODEL

Pascal Alexander Happ[1] and Romana Piat*[1]

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ABSTRACT

The development of new and for a specific application optimized particle reinforced composites usually necessitates a costly development process. Great advancements in this field were achieved by utilizing the growing computational powers into the development process and utilized methods such as FEA and analytic methods such as Mori-Tanaka, Lielens and the Self-Consistent Method [1]. The quality of the predictive models were increased by incorporating ever more detailed approximations of the studied particle shapes, resulting in increased computational expenses. The by the authors presented methods of combining the heuristic optimization method of Particle Swarm Optimization [2] with the combination with the generation of surrogate models of complex particle shapes is set to reduce and even enable the computational evaluation of the contribution of different particle shapes on the effective material properties of particle reinforced composites. Particle surrogate models with greatly reduced complex shapes in contrast to the exact particle shapes are generated by utilizing a sphere in combination with on top stacked layers. The material properties of each layer is then evaluated by employing the Particle Swarm Optimization method, which finds the optimal engineering constants for each layer by comparing the resulting effective material properties of the whole composite utilizing the surrogate particle model with the effective material properties of the composite utilizing the exact particle model. This optimization procedure has been carried out for reference volume elements with only one embedded particle, the resulting surrogate particles with the optimized engineering constants have afterwards been employed for reference volume elements containing multiple particle inclusions. Numerical simulations were firstly carried out for 2D particle shapes, as multiple exact particle inclusions could only be evaluated in the 2D case due to the high computational cost of modeling and evaluating multiple complex shapes in 3D. The here proposed methodology was then adapted for the 3D case, enabling the evaluation of the effective material properties of complex particle shapes.

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Inverse and optimization problems for advanced materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADVANCING INTEGRATED SILICON PHOTONICS: TOPOLOGY OPTIMIZATION OF MODE CONVERTERS AND SPLITTERS

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ABSTRACT

Integrated photonics design requires solving a massive number of degrees of freedom and ensuring fabrication viability with structural integrity. Inverse design tools like topology optimization, can yield non-continuous electromagnetic structures with extremely small features that are challenging to fabricate. The figure of merit depends on the tradeoff between design dimensionality, device footprint, functional complexity, and computational cost. In this study, we present a density-based topology-optimization framework to minimize the field overlap integral and obtain efficient designs simultaneously, ensuring fabrication. We adopt a new method of updating the binarization hyperparameters and a final smoothing to ensure physically realizable material from intermediate densities. Several numerical examples are presented to demonstrate the efficacy of the proposed method.

Advances in numerical methods for solution of PDEs
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MESH OPTIMIZATION AND BASIS COMPRESSION FOR EXTREME-SCALE SOLUTION OF PARTIAL DIFFERENTIAL EQUATIONS

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ABSTRACT

As computing technology moves toward utilizing accelerators with little onboard memory, traditional finite element methods (FEMs) must be adapted in order to fit extreme-scale simulations on fixed resources. One of the main challenges is evaluating and storing basis values for extreme numbers of basis functions. Methods such as sum factorization handle the polynomial degree scaling of those costs, but depend on geometry and choice of finite element basis. As an alternative, we introduce an approach that compresses the physical FEM basis values using measures of mesh cell similarity. Our approach may be used separately or complementary to sum factorization methods. Our compressibility metrics involve Jacobians of the reference-to-physical cell mappings, allowing for broad applicability to simplicial or tensor-product geometry and many finite element bases. When two different mesh cells are similar in shape, the reference-to-physical Jacobians are similar; therefore, the FEM basis values are also similar, and thus do not need to be re-evaluated. The errors made by this approximation may be characterized by considering the transforms specified by de Rham complex. Compressing these basis values allows for greater throughput in evaluating function values while reducing the memory overhead of the simulation. This compression may be additionally improved by performing R-adaptive mesh optimization offline using trust region augmented Lagrangian sequential quadratic programming algorithm [1], which moves mesh nodes so that the mesh cells have more similar shapes. To validate the theory, we present a variety of results related to the approximation quality, mesh optimization, performance metrics, and how one may use this approach to simulate 1 billion mesh cells on a single node of a typical supercomputer.

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Advances in neural operators for scientific modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

WATER WAVE EVOLUTION AND EQUATION DISCOVERY THROUGH NEURAL NETWORKS AND MACHINE LEARNING

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ABSTRACT

Despite research into water wave modeling and wave-structure interaction modeling over the decades, there remain many unknowns for even simply-stated cases under strongly nonlinear steep or breaking waves. For example, much work has recently focused on establishing a (potentially) universal breaking criterion. Meanwhile, machine learning techniques have developed to the point of standardizing equation discovery, either in the form of a neural network, or an interpretable equation. Application of the SINDy algorithm on known solutions to water wave propagation easily allows for the Korteweg-De Vries (KdV) equations to be found, an approximation in the weakly nonlinear, weakly dispersive limit. In this work, this is further developed in the time-domain, based on experimental data of irregular steep and breaking waves. Multiple approaches are compared, with a focus on steep unidirectional water waves. Comparison with classical weakly nonlinear surface reconstruction shows advantages.

Contact and interface mechanics: Modeling and computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN INTERIOR-POINT MULTIGRID BASED APPROACH FOR LARGE-SCALE CONTACT MECHANICS

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ABSTRACT

A critical aspect of modeling complex engineering systems is the interaction of physical bodies in contact. A number of frictionless contact problems have the property that the modeled state is the minimizer of an energy objective functional. However, generally such problems are: nonlinear, nonconvex and contain an optimization variable whose dimension is unbounded with respect to mesh refinement. We focus on the scalable solution of such large-scale contact mechanics problems on high-performance computing systems. We employ a Newton-based interior-point filter line-search method, that has emerged as one of the most robust methods for nonlinear nonconvex constrained optimization, to computationally estimate minimizers of such large-scale constrained optimization problems. The outer Newton-based interior-point loop converges rapidly; however, each step requires the solution of a large saddle-point linear system. A major challenge with the inner interior-point Newton-based linear system is that, in addition to the general challenges of solving large-scale linear systems, it can become arbitrarily ill-conditioned as the optimizer estimate approaches the optimal point. There are blocks that are amenable to multigrid which is a problem feature that we exploit. In this talk, we detail an interior-point multigrid-based approach for solving such problems and present scaling results obtained from an implementation of said framework on a few contact mechanics example problems. The results show that the solution of various contact mechanics problems can be achieved in a manner that scales well in the large-scale regime.

Isogeometric methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MACHINE LEARNING DISCOVERY OF OPTIMAL QUADRATURE RULES FOR ISOGEOMETRIC ANALYSIS

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ABSTRACT

We propose the use of machine learning techniques to find optimal quadrature rules for the construction of stiffness and mass matrices in isogeometric analysis (IGA) [1]. We initially consider 1D spline spaces of arbitrary degree spanned over uniform and nonuniform knot sequences, and then the generated optimal rules are used for integration over higher-dimensional spaces using tensor products. The quadrature rule search is posed as an optimization problem and solved by a machine learning strategy based on adaptive gradient-descent. However, since the optimization space is highly nonconvex, the success of the search strongly depends on the number of quadrature points and the parameter initialization [2]. Thus, we use a dynamic programming strategy [3] that initializes the parameters from the optimal solution over the spline space with a lower number of knots. With this method, we found optimal quadrature rules for spline spaces when using IGA discretizations with up to 50 uniform elements and polynomial degrees up to 8, showing the generality of the approach in this scenario. For nonuniform partitions, the method also finds an optimal rule in a reasonable number of test cases. We also assess the generated optimal rules in two practical case studies, namely, the eigenvalue problem of the Laplace operator and the eigenfrequency analysis of freeform curved beams, where the latter problem shows the applicability of the method to curved geometries. In particular, the proposed method results in savings with respect to traditional Gaussian integration of up to 44% in 1D, 68% in 2D, and 82% in 3D spaces.

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Modeling, optimization and computational analysis of metamaterials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SOME UNRESOLVED ISSUES IN TRUSS-LIKE MICROSTRUCTURE MATERIAL DESIGN

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ABSTRACT

Abstract
This article addresses long-standing misconceptions and misapplications in the field of material design by employing the mathematical theory of asymptotic homogenization (AH) and its substitutes [1]. One prevalent approach, persisting in the literature for approximately three decades, involves using the truss and frame cell of periodicity as the base building block of materials [2]. It is shown that using AH to design truss-like cellular composites is a misconception and unachievable. In this context, the flaws in a couple of notable articles that proceed with this approach are explained.
Additionally, the prevalent alternative approaches for imposing the unit initial strain and the periodicity boundary conditions to the base cell are scrutinized and the common flaws are elucidated. The article also briefly touches upon alternative energy methods. Another debated issue is the inconsistency between the bending action of beam members in frame microstructures and the assumption of cell periodicity. Also, common problems and misapplications related to alternative methods for AH in periodic truss and frame microstructures are addressed along with issues of truss nomenclature and finite element misapplications. Finally, some problems related to the recent artificial intelligence-assisted methods are briefly discussed [3].
Recognition of these problems is important, as they potentially impact energy, resource, and effort consumption.

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Smart structures – Modelling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ELEMENT-TYPE ANALYSIS FOR PLANAR ROTATING SQUARE AUXETICS—A FINITE ELEMENT STUDY

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ABSTRACT

Planar auxetic structures are commonly simulated using 2D elements in a small deformation regime to reduce computational costs. In this study, we conduct an element-type analysis on rotating square auxetics subjected to in-plane tensile loads within a large deformation regime to assess the validity of the 2D assumption. Four types of elements are selected, including plane stress, plane strain, shell, and 3D brick elements. The finite element (FE) results are then compared with experimental test results to identify the element that accurately represents the behavior of a rotating square auxetic. It was observed that, unlike small deformation regime, due to considerable through-the-thickness stress and strain, the 2D assumption is inadequate and fails to predict the actual behavior of the auxetic structure under large deformation conditions.

A HYPER-REDUCED ORDER MODEL FOR NONLINEAR COUPLED POROUS MEDIA FLOW

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ABSTRACT

The real-time simulation of complex geomechanical processes, such as hydraulic well stimulation, is computationally expensive since such systems often involve nonlinear and time dependent coupled thermo-hydro-mechanical equations. Finite Element Method (FEM) or similar methodologies can be utilized for the online (real-time) use or parameter estimation using field data; however, the simulation of large models often takes many hours to days. In this presentation, intrusive Model Order Reduction (MOR) techniques are developed for a system of nonlinear hydro-mechanical coupled equations to reduce computational costs. We will discuss various Reduced Order Models (ROM), including the need for a Proper Orthogonal Decomposition-Galerkin (POD-G) to reduce the number of degrees of freedom (DoFs), the need for Discrete Empirical Interpolation Method (DEIM) to accelerate the computation of nonlinear terms, and the need for local DEIM (LDEIM) [1] to apply a further reduction for nonlinear coupled transient problems. The ROM is carried out in an offline-online decomposition. First, some Full Order Models (FOMs) are carried out through a computationally offline stage to create a ROM basis. Then, through an online stage, full-physics FEM formulation will be improved by utilizing MOR formulations, and the trained MOR is employed to predict the response of the system. This presentation is built on our recent work on nonlinear porous media flow problems with time-discontinuous fluid injection rates [2]. Offline training of ROMs and online performance will be discussed for a two-dimensional analysis of hydraulic well stimulation, where a deformable porous medium is saturated with a single-phase fluid flow. The speed-up time and accuracy of ROMs are compared with coupled FOM. We will show that POD with LDEIM produces ROMs with accuracy comparable to FOM that execute significantly faster than FOM. In addition, an application of the presented ROM to a parameter sensitivity analysis is demonstrated. In this case, ROMs are parameterized from injection rate, permeability, and elastic parameters. It is demonstrated that the parameterized ROM can accurately reproduce deformation and pressure around the borehole.

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Immersed-boundary variational methods: Theory, data structures, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PARAMETER-ROBUST UNFITTED FINITE ELEMENT METHODS FOR A MAXWELL INTERFACE PROBLEM

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ABSTRACT

Geometrically unfitted finite element methods such as CutFEM, Finite Cell, XFEM or unfitted DG methods have been developed and applied successfully in the last decades to a variety of problems ranging from scalar PDEs on stationary domains to systems of PDEs on moving domains and PDEs on level set surfaces. These approaches combined with established tools of finite element methods allowed to apply and analyse unfitted methods in many fields. In this talk, we deal with an elliptic interface problem for the time-harmonic quasi-magnetostatic Maxwells equations.

Here the material function μ, the magnetic permeability, can jump at an interface.
Such problems are considered in low-frequency applications. Standard unfitted Nitsche methods are not robust with respect to the parameter k. For example, a standard Nitsche discretization for the curl-curl-operator introduces terms that do no longer vanish for gradient fields. In this talk, we will use a vectorial finite element discretization based on H(Curl) conforming functions. We will tackle the problem of robustness by introducing a scalar potential into the Nitsche formulation and thus apply a careful tailored ghost penalization term.

Computational methods for wind energy
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DESIGN OF WIND TURBINE DIFFUSERS USING STABILIZED METHODS AND THE VMS TURBULENCE MODEL

Hector Sanchez[1] *and Guillermo Hauke**[1]

[1]*EINA*

ABSTRACT

Harvesting the most of the wind resources presents a challenge in wind turbine devices and an important contribution towards the zero emissions objective. It has been shown that, for a given upstream flow conditions, diffusers augmented wind turbines (DAWT) present an opportunity to increase energy production of wind turbines [1]. The design of these devices will be addressed for a horizontal axis wind turbine using stabilized methods, MRF algorithms for fluid-structure interaction [3] and VMS turbulence models [2]. Some geometries that increase the wind harvested kinetic energy will be shown and the performance of the devices will be compared without and with a turbine rotor.

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Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A REVIEW OF VMS A POSTERIORI ERROR ESTIMATION IN COMPUTATIONAL FLUID DYNAMICS

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[1]*EINA*

ABSTRACT

VMS theory [1] was initially developed to evince the origins of stabilized methods. In this talk it is shown that stabilization parameters and stabilization terms contain true error information that can be used to obtain explicit and implicit a posteriori error estimates. The technology consists of splitting the exact solution into resolved or coarse scales (finite element solution) and unresolved or fine scales (numerical error). By feeding this splitting into the variational formulation, an exact weak form can be derived for the fine scales as a function of the resolved scales. The way of solving or approximating this equation yields different algorithms and models for error estimation [2]. Furthermore, using the so-called fine-scale Green's function, an analytical representation of the fine scales is possible. Different approximations of this function give rise to various algorithms and models. VMS theory naturally suggests that the error can be computed by the combination of element interior and inter-element faces residuals with the corresponding error time-scales. This technology can be further used for example to generate adapted meshes, to derive reduced order models and in verification and validation algorithms.

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Advances in computational biomechanics and mechanobiology
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MECHANICAL ANALYSIS OF CELL MIGRATION USING A STRUCTURAL OPTIMIZATION APPROACH

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ABSTRACT

The goal of this research is twofold that will provide predictive measures of two features of cell mechanics during their directed migration. The first goal is to exploit the use of modern optimization techniques in order to predict the orientation and size of actin stress fibers within the cytoskeleton. The second goal is to quantify the traction forces at these focal adhesion sites through these stress fibers during cell migration. For both scenarios, the cells are subject to a finite actomyosin supply constraint. The experimental measurements of such structural assembly inside the cell during migration is currently unavailable due to the limitations of modern microscopy, specifically because of our inability to image the cells at very high spatiotemporal resolution limited by photobleaching. A structural optimization framework can provide the predictive measure which is otherwise impossible by experimental means. Using this framework further, the quantification of the traction forces during migration is also quantified, which plays a crucial role in cell-matrix communication via mechanosensing. These results can be compared with the traction forces obtained by experimental methods, such as traction force microscopy. The benefit, however, of such a biophysical model as compared to experimental results, is that the parameters of the model can be adjusted to obtain new data regarding cell motion without having to rely on experimentation. The approach utilized here harness the power of modern structural optimization and optimal control. Structural optimization has proved to be a powerful method of generative design. However, the focus of the field has been on static structures, with exceptions to frequency-based structural optimization. Fully dynamic structural optimization has not extensively been studied since most systems do not possess the capability to generate their structural components over time. Therefore, with the power of structural optimization, nonlinear and optimal control theory, combined with the finite element method, a novel dynamic model of cell migration is achieved. He results might provide new methodologies and insights to the biomechanics and applied optimization research communities.

Recent advances in discretization techniques for coupled problems in incompressible fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE PICARD-NEWTON ITERATION FOR THE BOUSSINESQ EQUATIONS

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ABSTRACT

We propose, analyze and test the Picard-Newton iteration for the Boussinesq equations. The Picard-Newton iteration was (seemingly) recently developed as a two step method defined by a Picard step followed by a Newton step. We show this iterative method is an improvement on Newton that retains the quadratic convergence rate but has a larger basin of convergence. This is further improved by introducing Anderson Acceleration into the Picard step, and little seems to be lost when resolving the Picard step to only low accuracy.

Computational mechanics of soft matter and machines
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MECHANICAL-ELECTROCHEMICAL BEHAVIORS OF GEL ELECTROLYTE

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ABSTRACT

Wearable electronic devices and skin sensors require specific energy storage systems that combine high energy density and rate capability as well as long cycle life with additional features, such as high flexibility, high safety and environmental friendliness.[1] Flexible batteries based on hydrated polymer quasi-solid-state electrolytes (SSEs) are considered as promising solutions in view of their favorably high ionic conductivity and excellent flexibility. The rate capability and capacity retention of such flexible wearable batteries is controlled by the electrochemical and mechanical properties of the SSEs as well as their interfaces with the electrodes. Therefore, it is crucial to advance the development of new SSEs with wide electrochemical window, high stability and excellent mechanical strength in order to enable competitive wearable batteries.

In this work, a novel Zn2+ hydrogel polymer electrolyte has been synthesized, which achieves a high ionic conductivity of 4.8 × 10-4 S cm-1 at room temperature, and practically no change of conductivity up to 40 °C. Moreover, it features a wide electrochemical window ranging from 0 V to 2.06 V (vs. Zn/Zn2+). The mechanical strength of the electrolyte has been significantly enhanced from 0.6 MPa to 1.7 MPa by incorporating low-cost coconut fibers. Zn batteries employing our electrolyte achieve high capacity (80% of theoretical capacity) and maintain high stability and reversibility (99% capacity retention over 500 cycles at 5 C). The novel flexible battery has also been demonstrated to function with outstanding performance over the relevant temperature range down to low temperatures (4 °C) as well as under bending, meeting the key criteria for flexible power supply in wearable electronic devices.

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Smart structures – Modelling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DYNAMIC DISPLACEMENT RECOGNITION OF FRAME STRUCTURES BASED ON COMPUTER VISION

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ABSTRACT

The safety of engineering structures has increasingly become a concern, and the rapid assessment of structural safety has become a focal point and challenge in this field. With the development of structural health monitoring technology and the emergence of intelligent tools such as computer vision, research on real-time health monitoring of structures that combines both contact and non-contact methods holds significant theoretical significance and engineering application value. The displacement of a structure under external forces is one of the more intuitive variables for structural safety assessment. Traditional contact methods, such as placing displacement sensors on structures, are often constrained by objective factors. Non-contact methods, like utilizing computer vision algorithms such as optical flow estimation and feature matching, can rapidly and accurately obtain structural displacement. They also offer advantages such as being unaffected by the structure itself and having quick deployment. However, improving the accuracy of displacement monitoring based on computer vision is a key focus in this research field. This paper proposes a data processing method for dynamic displacement in structures based on a combination of non-contact and contact approaches. It fuses dynamic displacement identified through computer vision technology with data recorded by acceleration sensors on the structure to enhance displacement monitoring accuracy.

Firstly, a multi-target template matching algorithm based on OpenCV is used to convert the dynamic trajectories of known feature points on the structure into pixel displacements. The dynamic distances of feature points identified by template matching are used to calculate a scaling factor based on known structure dimensions. Secondly, the displacement converted from acceleration sensor data is fused with pixel displacement upsampled to the same frequency as the sensor through Kalman filtering. This process simulates the real displacement of the structure. Finally, the random subspace method is employed for structural modal parameter identification, validating the feasibility of the approach proposed in this paper. The research results indicate that this method can obtain dynamic structural displacement based on computer vision information. The relative error in monitoring data is reduced from 43.75%, as seen in traditional methods, to an average of 7.46%, demonstrating the effectiveness and reliability of the proposed approach.

Data-driven approaches for solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NEURAL NETWORK ENHANCED DIFFERENTIABLE MESHFREE METHOD FOR COMPUTATIONAL MECHANICS

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ABSTRACT

Physics-informed/physics-constrained machine learning approaches have received increased attention for solving both forward and backward computational mechanics problems across diverse engineering applications. However, their predictive accuracy and training efficiency encounter limitations in realistic engineering scenarios, especially those involving kinematic and material nonlinearities. In this presentation, we introduce a newly proposed differentiable meshfree approach--the neural-integrated meshfree (NIM) method [1]. NIM is derived based on a hybrid neuro-numerical approximation, facilitating the efficient training of neural networks while adhering to the underlying governing equations within a consistent meshfree Galerkin framework. The numerical results of several benchmark examples, including stationary and transient mechanics problems, showcase the enhanced performance of NIM in terms of accuracy, scalability, and convergence properties. In addition, we extend the NIM framework to model inelastic materials, where the effects of different loss function formulations on encoding internal state variables and nonlinear material laws are investigated. To highlight the superior performances of the proposed method against existing approaches in the literature, several inelastic material models are considered in the study.

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Deep and machine learning methodology in the context of application to computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICS-INFORMED NEURAL NETWORK IN PARTIAL DIFFERENTIAL EQUATIONS FOR FINITE ELEMENT ANALYSIS OF FLASH SINTERING

Ran He[*1], Mingxuan Xia[1], Peter Polak[1], Baber Saleem[1], Michael Yu[1], Xiaoxia Yu[1] and Jingzhe Pan[1]*

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ABSTRACT

Flash sintering is characterised by the application of an electrical field to a material body during sintering. This method achieves remarkable heating rates by directly dissipating heat within the ceramics, significantly reducing both processing time and furnace temperature compared to the conventional sintering. This enhancement leads to increased throughput and productivity, marking a notable improvement in the processing efficiency. However, flash sintering presents specific challenges, particularly in controlling deformation and grain growth. This challenge can occur as a result of the resistive heating caused by the applied electric current. To achieve the desired final shape of the material, accurately predicting the temperature distribution in the sintering part is critical. Currently, the Maxwell's functions and heat equation are used to simulate the fields of electricity and heat in the finite element analyses. However, they may not fully capture the actual fields. To address this challenge, this study aims to introduce a new backpropagation strategy for an artificial neural network (ANN) to replace ohmic heating due to electric current in the heat equation for the finite element analysis, and, thus, to accurately predict the temperature distribution and sintering behaviour of the sintering part.

This innovative approach involves a two-step training process for the ANN. The inputs consist of current, temperature and relative density, with the ohmic heating as the output. Firstly, the ANN is trained to learn the relationship between the ohmic heating and the applied electric current based on the existing developed equations. This trained ANN is implemented in COMSOL to simulate the process of flash sintering. Its results are compared with those simulated by the existing equations, showing a good agreement. Subsequently, the ANN is retrained with experimental data. As the experimental data are only available for the surface temperature of the sintering part, not the ohmic heating, the loss function is defined as the mean squared error of the surface temperature instead of the ohmic heating. Hence, a new backpropagation strategy is developed with its mathematical prove. The retrained ANN is again implemented in COMSOL to simulate the process of flash sintering. The simulated temperature and relative density are in good agreements with the experimental data. This validates the feasibility of the proposed backpropagation strategy to replace a parameter/term in the partial differential equation in the finite element analysis of flash sintering.

Recent advances in computational fracture mechanics and failure analysis
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

S-VERSION FEM-BASED STRATEGY FOR SIMULATING HIGH-SPEED CRACK PROPAGATION BEHAVIOUR IN 3D STRUCTURES

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ABSTRACT

Developing a numerical method to simulate the brittle crack propagation behaviour accurately and efficiently is crucial for ensuring the safety of large-scale engineering structures. This study proposed a novel strategy based on the s-version finite element method (s-method) for simulating high-speed crack propagation in 3D structures.

In the proposed strategy, the high-speed crack propagation is modelled by a combination of the nodal force release method and local mesh update. The global mesh is generated based on the entire domain geometry without considering crack propagation, which significantly simplified the mesh generation procedure. Meanwhile, the local mesh is generated only in the vicinity of the crack front with fine elements to ensure high accuracy. However, ensuring complete coverage of the target domain necessitates extending the local mesh beyond the surface of the 3D structure. Such an incompatibility between the surface of the target domain and boundaries of the local mesh causes non-negligible errors in the conventional s-method. To address this issue, we propose an approach based on Heaviside enrichment to eliminate these errors.

The proposed strategy was initially verified by evaluating the accuracies of the local stress in stationary and dynamically propagating circular crack in a 3D solid, as well as those of the stress intensity factor. The results demonstrate that the proposed strategy provides unprecedented accuracy and efficiency of local stress evaluation in problems of dynamic crack propagation without requiring any complicated remeshing procedures.

Subsequently, to further validate the effectiveness of the proposed strategy for simulating the high-speed crack propagation in real engineering structures, numerical examples to analyse the experimental results of high-speed crack propagation in double cantilever beam-type plate and joint specimens made of polymethyl methacrylate (PMMA) are presented. The numerical results demonstrated the effectiveness of the proposed strategy for simulating high-speed crack propagation in 3D structures. Consequently, the proposed strategy has the potential to serve as a fundamental numerical framework for simulating dynamic crack propagation in engineering structures.

RESEARCH ON AIRCRAFT TIRE SPRAY PROBLEM ON WET RUNWAY BASED ON IMPROVED SPH ALGORITHM

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ABSTRACT

Abstract
The tire-generated water spray may enter the engine when the aircraft takes off or lands on the wet runway, and lead to the compressor stall, surge, or even combustion flame-out. Therefore, to study the problem of aircraft tire spray is of great significance to the safety and the airworthiness certification of the aircraft. Based on the self-developed SPH program, the problem of aircraft tire spray will be researched thoroughly by the combination of experiment and numerical simulation in this paper. When simulating this kind of fluid-elastomer interaction problem with traditional SPH (Smoothed Particle Hydrodynamics) method, there are some drawbacks in both fluid and elastomer calculation. For the elastomer simulation, the TL-SPH (Total Lagrangian-SPH) is used to deal with the deformation of tire under complicated motion and load. For the fluid simulation, the Riemann SPH combined with transport velocity technology is proposed to solve the problem of tension instability in free liquid surface splashing. On this basis, the SPH model of tire spray is established. By carrying out the aircraft tire vertical water entry experiment, the morphological characteristics of the tire spray are captured. The morphological description method is determined. These provide the verification basis for the numerical calculation. Then, the formation mechanism of spray is analyzed by numerical simulation. Finally, based on the large-scale tire spray simulation, the phenomenon of tire hydroplaning is studied, and the causes of hydroplaning phenomenon and its influence on spray form are analyzed.

Keywords: SPH (Smoothed Particle Hydrodynamics), aircraft tire spray, fluid-structure interaction, tensile instability.

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Nanomechanics and nanoscale thermal transport for new materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A PERIDYNAMICS MODEL FOR THE FRACTURE IN GRAPHENE SHEETS

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ABSTRACT

This work establishes an ordinary state-based peridynamic coarse-graining (OSPD-CG) model based on the interatomic potential at nanoscale to study the fracture in nano-materials, i.e. the fracture in graphene sheets (GS). The PD model for linear elastic solids is generalized as a nonlinear one to model fracture in physical nonlinear materials, i.e. GS. Based on energy conservation, the PD parameters are derived from full atomistic molecular dynamics (MD) simulations in which interatomic potential is used. The PD model is verified by comparing the Young's modulus calculated from PD and the one from MD. The PD simulation results such as the stress-strain relations and the crack propagation patterns are also compared with those from full atomistic MD simulations to show the validity of the PD model. The fracture mechanisms in GS are revealed as well. For example, the primary crack branches into two secondary cracks after propagating straightforward for a short time at initial stage. Then the secondary cracks keep propagating near the boundaries and their propagating directions are changed due to the influence of the boundaries. And in the propagation process of secondary cracks, some micro-cracks even tertiary cracks generate due to the branching of secondary cracks. Furthermore, this work also shows the advantage of the OSPD-CG model here over MD simulations that the current model can be used to study larger scale systems with higher efficiency.

Keywords: Ordinary State-based Peridynamics; Molecular dynamics; Crack propagation; Graphene

Advances and applications of polytopal methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A TPAA-MSSBFEM FOR SOLVING NONLINEAR TRANSIENT HEAT TRANSFER PROBLEMS OF TWO-DIMENSIONAL HETEROGENEOUS MATERIALS

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ABSTRACT

By combining the Multiscale Scale Boundary Finite Element Method (MsSBFEM) and the Temporally Piecewise Adaptive Algorithm (TPAA), a new numerical model is presented to reduce the solution scale of the two-dimensional heterogeneous nonlinear transient heat transfer problems. Utilizing TPAA, a spatially and temporally related problem is transformed into a series of recursive spatial problems, which are solved by MsSBFEM. The solution scale can be effectively reduced by recourse of a bridge between small-scale and large-scale via quadtree Scaled Boundary Finite Element Method (SBFEM) based numerical base functions. In the spatial domain, utilizing the advantages of image-based quadtree gridding, the construction of numerical base function can be conveniently and efficiently conducted particularly for the heterogeneous media with complex geometries at the small-scale. In the updating of numerical base function in the nonlinear multiscale computation, combine with the reduced integration method, the sparse transition quadtree mesh with the fixed element pattern makes the solution of nonlinear heat transfer problem and updates of numerical base function more efficient. The adaptive updating criterion of the numerical base function is proposed, which further improves the computational efficiency of multiscale analysis. The TPAA can maintain temporal computational accuracy via an adaptive process when the step size varies. Numerical examples are provided to elucidate the effectiveness of proposed approaches, and satisfactory results are achieved at both the large and small scales.

MONOLITHIC MULTIGRID FOR THE MARKER-AND-CELL DISCRETIZATION OF THE STOKES--DARCY EQUATIONS

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ABSTRACT

In this talk, we consider the marker-and-cell scheme for numerically solving the Stokes--Darcy equations. The corresponding discrete system has a double saddle-point structure. Designing a fast solver for such a problem is challenging due to the different scale of the physical parameters. We propose a monolithic multigrid solver with a block-lower-triangular smoother based on the block-LU decomposition of the coefficient matrix, which requires solving a Poisson-type equation with a scalar Laplacian and two Schur complement systems. We demonstrate the robustness of a sparse approximate inverse smoother for the Laplacian, and we handle the Schur complement systems by applying simple relaxation schemes as smoothers. The proposed scheme is economical, and yet it is robust with respect to the mesh size and the physical parameters.

Fracture, damage and failure mechanics of cementitious materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CALIBRATION OF DAMAGE PARAMETERS OF SUPER HIGH-RISE FRAME-CORE STRUCTURAL SUBSYSTEM UNDER TORSIONAL GROUND MOTION

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ABSTRACT

The super high-rise frame-core tube structure consists of multiple subsystems that collectively respond to torsional seismic action. The damage progression and failure of multiple subsystems have a direct impact on the seismic safety of the structure. However, current torsional control methods primarily address the torsional regularity of the entire structure, while overlooking the impact of the torsional component of ground motion and the torsional damage within internal subsystems. The characterization of torsional damage in the subsystem subjected to torsional ground motion provide support for subsequent analysis of translation-torsional coupled damage. To elucidate the dynamic characteristics of the structure under torsional excitation, this paper derived the torsional vibration equation for the structure and the restoring force model for each subsystem. The accuracy of the dynamic model was then verified through a combination with the finite element model. To choose a suitable damage index that accurately describes the torsional damage degree of the subsystem, while taking into account the applicability of stiffness degradation to both the overall structure and each subsystem, the stiffness degradation coefficient was identified as the key index to depict the damage degree of each subsystem after the structure enters the elastoplastic stage. Moreover, acknowledging the limitations of the current method for estimating stiffness degradation coefficients, the NSGA-II genetic algorithm was employed in this study. The initial stiffness and yield strength of each subsystem serve as optimization variables in the design of a comprehensive optimization plan that considers both structural cost and overall torsional damage. Considering the time-consuming nature of elastic-plastic time history analysis, an independent torsional pushover analysis method was developed and validated using time history analysis. By introducing reasonable assumptions, the optimization example was designed to preserve solely the simplified structure of the reinforcement layer. Meanwhile, due to the difficult of considering the plastic development of the outrigger truss in the plane with the rigid floor slab assumption, the assumption of concentrated plastic hinges was applied at the connection between the outrigger and the column end. The hysteresis parameters of each subsystem in the optimization example align with those mentioned above. The validity of the assumed hysteresis parameters was confirmed through torsional pushover analysis of the optimization examples. A reasonable estimation of the stiffness degradation coefficient was obtained by incorporating the Q-hysteresis model.

Computational mechanobiology of musculoskeletal tissues
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HOW OSTEONS FORM: A QUANTITATIVE HYPOTHESIS-TESTING ANALYSIS OF CORTICAL PORE FILLING AND WALL ASYMMETRY

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ABSTRACT

Osteon morphology provides valuable information about the interplay between different processes involved in bone remodelling. The correct quantitative interpretation of these morphological features is challenging due to the complexity of interactions between osteoblast behaviour, and the evolving geometry of cortical pores during pore closing. We present a combined experimental and mathematical modelling study to provide insights into bone formation mechanisms during cortical bone remodelling based on histological cross-sections of quiescent human osteons and hypothesis-testing analyses. We introduce wall thickness asymmetry as a measure of the local asymmetry of bone formation within an osteon and examine the frequency distribution of wall thickness asymmetry in cortical osteons from human iliac crest bone samples from women 16–78 years old. Our measurements show that most osteons possess some degree of asymmetry, and that the average degree of osteon asymmetry in cortical bone evolves with age. We then propose a comprehensive mathematical model of cortical pore filling that includes osteoblast secretory activity, osteoblast elimination, osteoblast embedment as osteocytes, and osteoblast crowding and redistribution along the bone surface. The mathematical model is first calibrated to symmetric osteon data, and then used to test three mechanisms of asymmetric wall formation against osteon data: (i) delays in the onset of infilling around the cement line; (ii) heterogeneous osteoblastogenesis around the bone perimeter; and (iii) heterogeneous osteoblast secretory rate around the bone perimeter. Our results suggest that wall thickness asymmetry due to off-centred Haversian pores within osteons, and that nonuniform lamellar thicknesses within osteons are important morphological features that can indicate the prevalence of specific asymmetry-generating mechanisms. This has significant implications for the study of disruptions of bone formation as it could indicate what biological bone formation processes may become disrupted with age or disease.

Modeling and simulation of coupled processes in geological media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING OF PDC CUTTER – ROCK INTERACTIONS USING HOSS

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ABSTRACT

Polycrystalline diamond compact (PDC) cutters are used in geothermal energy drilling operations as they are especially effective due to their resistance to abrasion and strength. It is important to understand the effect of downhole conditions on the bit to accurately model PDC cutter - rock interactions and drilling efficiency. When attempting to increase drilling or cutting efficiency, the time that the drill bit is not in contact with the rock is detrimental for the operation. Cutting efficiency is determined through the weight on the bit, rotational speeds, and other cutter and rock parameters that can be modeled. To accurately describe this interaction, we use the combined finite discrete element method (FDEM) to model the PDC cutter – rock interaction. FDEM can model both continuum and discontinuum (it’s never been clear to me if this is a real word?) mechanical behavior, cutter-rock interaction results in rock fracture and fragmentation, reproducing material behavior similar to targeted rock at downhole conditions. We use HOSS, an FDEM code, for our numerical studies.. We model the cutter as a rigid body acting on a granite block. One of the outputs of the simulations is the cutting force, which we use to understand cutting efficiency in the model. We study the interaction between the PDC cutter and the rock with and without pressure to get an understanding of rock fracturing processes on the surface and downhole. In this presentation we report on the progress of the numerical analysis for this complex multi-physics problem.

Numerical modeling of granular and multiphase flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFECT OF PARTICLE-SIZE-SCALING ON PARTICLE INTERACTIONS IN DEM-SIMULATIONS OF SAND IN THE CONTEXT OF AIR PLUVIATION

Natascha Heim[*1] and Sascha Henke*[1]

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ABSTRACT

DEM (discrete element method) is a widely used numerical simulation method, which models the behaviour of a bulk substrate based on the individual interactions of many particles. One of its possible applications is the modelling of sand behaviour in different laboratory test, for example cone penetration tests [1] or direct shear tests [2]. Furthermore, DEM is specifically of interest as a modelling method for investigating air pluviation, because it models the individual inter-particle and particle-environment interactions, both friction and collisions, which determine the compaction and homogeneity of the created samples.

However, one disadvantage of DEM is the relatively long computational time [3] especially with decreasing particle sizes. This makes larger particle sizes compared to reality more interesting, especially for large scale or repeating simulations. On the other hand, if the size of the chosen particles is too large, certain interactions, such as interactions with other materials and equipment, may not be simulated in a way that properly represents real behaviour. This would lead to preferring smaller sized particles, which again would lead to longer computational times.

Therefore, the chosen particle size as an important aspect of DEM simulations will be discussed, as well as the effects on different simulation aspects. This includes necessary parameter adjustments, the resulting inter-particle and particle-environment interactions as well as the achieved simulation results and accuracies. Of specific interest is the largest particle size, at which accurate and realistic results concerning real-world particle interactions can be achieved. Further, the effects of graded particle sizes to better represent the sand during the pluviation process will also be discussed.

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Recent advances in high-order methods for computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CAN HIGH-ORDER CONVERGENCE BE OBTAINED FOR PRACTICAL PROBLEMS IN ENGINEERING?

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ABSTRACT

With all of the interest in high-order methods, it is still not clear whether these methods have an advantage over their low-order counterparts for practical problems. In this talk, high-order hp-finite element moving mesh formulations for problems with moving boundaries and discontinuous solutions will be discussed. In particular, the attainable order of accuracy will be examined for several practical applications. These applications include ducted wind turbines where the rotor is modeled with an actuator disc, solidification of silicon with a moving free-surface and solidification front, and re-entry vehicles with a bow shock where the bow shock is tracked by the moving mesh. In all of these cases the solutions have non-smooth behaviors which makes obtaining design order of accuracy difficult / impossible. We examine whether high-order accurate schemes are still advantageous for these types of problems for both uniform mesh refinement approaches and adaptive meshing. We then investigate coordinate transforms that allow high-order methods to obtain optimal accuracy even for problems with singularities.

Fluid dynamics and SciML: Navigating challenges and seizing opportunities
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MESH MOTION WITH SCIENTIFIC MACHINE LEARNING

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ABSTRACT

Mesh motion operators are used in various applications, such as fluid-structure interaction (FSI) in the arbitrary Lagrangian-Eulerian (ALE) formulation or shape optimization with the method of mappings, to map a reference domain to a deformation of the domain. Typically, extension operators are defined by the solution of PDEs, with Dirichlet boundary conditions representing the deformed geometry, but PDE-based extension operators capable of handling large deformations can be prohibitively computationally expensive. Therefore, we investigate replacing these operators with data driven surrogates. Taking inspiration from the PDE nature of typical extension operators and the graph structure of meshes, we propose operator learning- and graph neural network-based methods, tailored for the specific application of learning mesh motion operators. We discuss aspects of network architecture, training, and implementation, evaluating the models as the ALE mapping in an FSI benchmark problem.

Geomechanics of the cryosphere
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ON SEA ICE DYNAMICS APPLYING MIXED LEAST-SQUARES FEM

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ABSTRACT

The behavior of sea ice has been studied for many decades. In order to model its viscous-plastic behavior at scales spanning several thousand kilometers, different numerical models have been proposed. Based on the established approach in [1], this contribution presents a simulation model for sea ice dynamics to describe the sea ice circulation and its evolution over one seasonal cycle. In course of that, the sea ice concentration and the sea ice thickness are considered, of which the physical behavior is governed by transient advection equations. Here, the sea ice velocity serves as coupling field.
Recently developed approaches base on a finite element implementation choosing a (mixed) Galerkin variational approach, see e.g. [2 and [3]. But therein, challenges may occur regarding the stability of the numerically complex scheme, especially when dealing with the first-order advection equations. Thus, we propose the application of the mixed least-squares finite element method, which has the advantage to be also applicable to first-order systems, i.e., it provides stable and robust formulations even for non-self-adjoint operators, such as the tracer equations (for sea ice thickness and sea ice concentration).
For solving the instationary sea ice equation the presented least-squares finite element formulation takes into account the balance of momentum and a constitutive law for the viscous-plastic flow. The considered primary fields are the stresses, the velocity. the concentration and the thickness. In relation, four residuals are defined for the derivation of a first-order least-squares formulation based on the balance of momentum, the constitutive relation for the stresses, and two tracer-equations. Different approaches can be made with respect to the approximation functions of the primary fields, i.e., choosing e.g. conforming (H(div) interpolation functions) or non-conforming (Lagrangian interpolation functions) stress approximations, while Lagrangian interpolation functions are chosen for the remaining fields. In order to compare such approaches, the box test case is utilized, cf. [3], which is well described in literature.

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Computational methods for wind energy
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

OFFSHORE WIND CLUSTER MODELING USING ANALYTICAL WAKE MODELS CALIBRATED USING LONG-TERM SCADA DATA AND SCANNING LIDAR

Diederik van Binsbergen[1], Pieter-Jan Daems[2], Timothy Verstraeten[2], Amir Nejad[1] and Jan Helsen[2]*

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ABSTRACT

Today, offshore wind farms are deployed in offshore concession zones. Such concessions are a cluster of multiple farms. The modeling of the wake effects of wind farms in such clusters cannot be limited to the single farm perspective. Deep array effects due to dense turbine spacing result in important significant internal wake effects, whereas closeness of the farms to each other causes non-neglectable external wakes. As such, it is necessary to have a physics-based model that can scale to the offshore wind farm cluster as whole. In literature multiple analytical wake deficit models are available to predict the individual power output of the turbines in the wind farm cluster. In recent years many research efforts were done resulting in novel model types such as Cumulative wake / curl, Turbopark, TurboGauss,… These recent modeling approaches aim to account better for these deep array effects and long spatial evolution of the wakes (far wakes). Furthermore, novel blockage modeling approaches were developed to describe the velocity deficit at the wind farm inflow due to the inertia effects of the large number of turbines in the cluster. This study aims to benchmark these different models on the Belgian offshore cluster consisting of >2GW of wind power. One year of SCADA data of 5 wind farms are used to calibrate the hyperparameters of the analytical wake models. Once calibrated the accuracy of the models is benchmarked on multiple years of SCADA data of the same 5 farms. With the performance metrics utilized in this work, it is shown that top-hat models perform relatively better compared to their Gaussian counterparts. This could be due to their overestimation of the wake deficit at the wakes' edge, which might indirectly account for wake meandering and wake steering due to turbine misalignment, compared to its Gaussian variant. Novel models, such as the TurbOPark and TurbOGauss models, furthermore, outperform their traditional counterparts (Jensen and the Gaussian model developed by Bastankhah and Porte Agel (2014) in scenarios where wakes propagate through highly varying turbine spacings, getting worse when turbine spacing increases. Additionally, a large performance increase is observed when the wake expansion rate is taken as a function of local turbulence intensity, as described in Niayifar and Porte Agel (2016). Furthermore, scanning lidar data from a multi-month offshore monitoring campaign at one of the farms is used to further validate and benchmark the models.

Verification techniques in computational physics and applied mathematics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN OVERVIEW OF SYMMETRY-PRESERVING NUMERICAL METHODS FOR VERIFICATION

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ABSTRACT

Symmetry-preserving numerical methods (SPNMs) are used for numerical approximations when a symmetry group of a system of differential equations is wished to be preserved. Generally speaking, these numerical methods can greatly reduce computational error compared to numerical methods that do not preserve symmetries[1]. SPNMs are used in a wide variety of applications, ranging from robotics to signal processing[2]. For verification, SPNMs may serve as standards for which other algorithms may be compared when analytic solutions are not known in order to determine an estimate of numerical error. We will give an overview of SPNMs and the specifics of how they may be used for verification purposes.

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Machine learning algorithms for accelerating material characterization, discovery, design, and manufacturing processes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN FRAMEWORK FOR THE ACCELERATED SCREENING OF HIGH-ENTROPY ALLOYS CATALYSTS

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ABSTRACT

High-entropy alloys (HEAs) have attracted significant interest in recent years due to their exceptional properties over conventional alloys. Recently, HEAs have shown remarkable catalytic performance especially for oxygen reduction reaction (ORR) and carbon dioxide reduction reaction (CO2RR). First principle calculation methods such as density functional theory (DFT) are typically used to explore active and stable electrocatalysts. However, the ability to use explore HEAs for catalytic application using conventional DFT is hindered by the vast configuration space due to the large number of possible arrangements of surface sites. This requires a huge number of DTF calculations, which can be infeasible. Machine learning (ML) approaches have been recently used for catalysis prediction. However, a significant drawback of ML is that large data sets are needed for training and validating the ML models. To tackle this issue, robust approaches to efficiently screen the configurational space of catalytic HEA materials need to be developed and employed. An efficient method to navigate the configuration space of HEA alchemical perturbation density functional theory (APDFT). A key advantage of APDFT is that a single Density functional theory (DFT) calculation of the adsorbate's binding energy (BE) can be used to predict many hypothetical catalysts surface structures' BE at a negligible additional computational cost. This characteristic makes APDFT an appealing technique to explore the configurational space of catalytic HEAs at significantly less computational cost. The accuracy of APDFT was assessed for different adsorbates on AuAgPtPdCu HEA surface. The results have shown that APDFT can capture the BE trends with minimal computational cost, suggesting a fast-screening approach with less number of brute-force DFT calculations required. Coupled with APDFT, ML were developed based on fewer computationally expensive DFT calculations, accelerating the screening of HEAs for catalysis applications. Our proposed framework is based on a Gaussian process regression (GPR) model using the data from APDFT calculations for training and validation sets. We propose to use a GPR model based on graph theory to describe the chemo-spatial environment of the adsorbate on HEA surface for BE prediction, coupled with the data from the data from APDFT calculations for training and validation sets. Here, since the model is trained and coupled with low-cost APDFT calculations, we explore millions of compositional spaces with the GPR at minimal cost. This allows to tune the HEA composition to obtain large number of sites with optimal binding energies which eventually can increase the catalytic activity for HEAs.

Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INVESTIGATION OF GEOTRIBOLOGICAL BEHAVIOUR IN THE SOIL-PILE INTERFACE CONSIDERING CLAY BASED ON NUMERICAL AND LABORATORY INVESTIGATIONS

Sascha Henke[1] and Philipp Wiesenthal*[1]

[1]*Helmut Schmidt University*

ABSTRACT

The contact behaviour between soil and structures is an important aspect in many geotechnical applications. One example is the contact between pile and soil during pile installation which especially for open-ended pipes can lead to soil plug formation.

Within the present research, contact behaviour between clayey soil and pile is investigated by means of numerical and laboratory experiments focussing on the contact behaviour within tubular piles.

First, the contact behaviour between kaolin clay and steel is experimentally investigated with respect to overburden pressure in the so-called Geo-Tribometer developed at HSU. As the results of the experimental investigations show some unexpected results leading to the assumption that the contact failure surface inside the soil specimen changes with differing overburden pressure. Additional numerical simulations are carried out for better understanding of contact stress development.

Second, further laboratory investigations using soil-filled tubular piles show that adhesion effects significantly influence the contact behaviour between soil plug and internal surface of the tube. For estimation of the adhesion values numerical simulations by means of finite element analyses are carried out showing for example that as expected with increasing soil’s pre-overburden pressure the adhesion effect increases.

The results are finally discussed with respect to transferability from the small scale in numerical and laboratory investigations towards prototype scale.

INVERSE UNCERTAINTY QUANTIFICATION IN PASSIVE AUTOMOBILE SAFETY: BAYESIAN INVERSION FOR OPTIMAL PASSIVE SAFETY AT FULL-VEHICLE SCALE

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[3]*appliedAI Institute for Europe*

ABSTRACT

We introduce an innovative approach to inverse uncertainty quantification in the domain of passive automobile safety, utilizing Bayesian inversion techniques. Our method computes the required input distributions of key safety variables to achieve a desired distribution in the results space. This proactive methodology shifts from a traditional trial-and-error to a question-oriented approach: “What adjustments are necessary to ensure optimal occupant protection?”, conceptualizing the target as a distribution rather than a fixed outcome. A central feature of our methodology is its ability to recognize alternative solutions, yielding similar results. Secondly, balancing between achieving extreme safety results and maintaining robustness under various conditions is addressed with a robustness metric to assess such solution sets. Additionally, the approach benefits from leveraging the analytical describability of certain parts of the safety engineering process. This reduces the size of the required data set and enhances the practicality of the method.
Distinctively, we demonstrate our method’s effectiveness on a full-vehicle scale industry problem, underscoring its scalability and real-world relevance. This demonstration confirms the feasibility of applying our approach in complex automotive safety scenarios. By integrating Bayesian inversion with a data-driven strategy and introducing a robustness quantification metric, our approach offers an efficient and versatile tool for enhancing the safety engineering and verification process in the automotive industry.

Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DISTORTION COMPENSATION FOR METAL ADDITIVE MANUFACTURING: VERIFICATION, VALIDATION, AND DEVELOPMENT OF A THERMAL MECHANICAL WORKFLOW

Carl Herriott[1], Michael Stender[1], Kyle Johnson[1], Jonathan Pegues[1], Christie Crandall[1] and Sannmit Shinde[1]*

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ABSTRACT

Additive manufacturing in metals has enabled the design and manufacturing of previously unthinkable geometries holding great promise for a wide range of manufacturing applications. Inherent to the additive manufacturing process in metals are residual stresses and distortions which can lead to as-built components not meeting geometric requirements. Mitigation and/or compensation for the combined effects of distortions and residual stresses is a critical step to enabling additive manufacturing in production-level critical structures.

To address the negative effects of residual stresses and distortions, an efficient thermal mechanical simulation-based distortion compensation workflow has been implemented. In this workflow, distortions and residual stresses are predicted for the purpose of an inverse analysis. This iterative workflow modifies the as-designed CAD geometries based on mapped distortions to successfully print a part to meet geometric requirements using an updated CAD geometry. Additionally, common post-processing steps, such as heat-treatment and baseplate removal, are simulated by the workflow to capture their impact on the distortion of the printed part.

This talk will discuss the details of workflow development and verification, sensitivities of this approach, and validation of model results against experimental data for a variety of builds.

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Theory and application of provably-robust and efficient high-order methods for high-fidelity computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STRONGLY STABLE DUAL-PAIRING UPWIND SUMMATION-BY-PARTS FINITE DIFFERENCE SCHEMES FOR THE VECTOR INVARIANT SHALLOW WATER EQUATIONS

Justin Kin Jun Hew[*1], Kenneth Duru[1], Stephen Roberts[1], Christopher Zoppou[1] and Kieran Ricardo[1]*

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ABSTRACT

We present an energy/entropy stable and high order accurate finite difference method for solving the nonlinear shallow water equations (SWE) in vector invariant form using the newly developed dual-pairing and dispersion-relation preserving summation-by-parts finite difference operators. We derive new well-posed boundary conditions for the SWE in one space dimension, formulated in terms of fluxes and applicable to linear and nonlinear problems. For nonlinear problems, entropy stability ensures the boundedness of numerical solution but does not guarantee convergence. Adequate amount of numerical dissipation is necessary to control high frequency errors which can generate artefacts in numerical simulations. Using the dual-pairing SBP framework, we derive high order accurate and nonlinear hyper-viscosity operator which dissipates entropy and enstrophy. The hyper-viscosity operator effectively tames oscillations from shocks and discontinuities and eliminates poisonous high frequency grid-scale errors. The numerical method is most suitable for the simulations of sub-critical flows typically observed in atmospheric and geostrophic flow problems. We prove a priori error estimates for the semi-discrete approximations of both linear and nonlinear SWE. We verify convergence, accuracy, and well-balanced property via the method of manufactured solutions and canonical test problems such as the dam break, lake at rest. Numerical simulations in two-dimensions are presented which include the rotating and merging vortex problem and barotropic shear instability, with fully developed turbulence.

Advances in computational mechanics for flow-induced vibrations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A HYBRID MODAL AND GRAPH NEURAL NETWORK ANALYSIS: APPLICATION TO FLOW-INDUCED VIBRATION OF LONG FLEXIBLE CANTILEVERS

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ABSTRACT

This study employs a numerical framework to investigate the sustained oscillations of a flexible cylindrical cantilever beam immersed in fluid flow. The flow equations are formulated within an arbitrary Lagrangian-Eulerian (ALE) framework, accounting for the moving boundaries of the structure. The fluid-structure interface is addressed through a partitioned iterative scheme, ensuring stable coupling of the Navier–Stokes equations with low-mass flexible structures experiencing strong inertial effects from the surrounding incompressible flow. The flexible cantilever is represented as a slender structure using linear modal analysis [1,2]. The current investigation focuses on key aspects of numerical modeling: (i) assessing the effectiveness of the modal analysis in capturing the flexible cantilever's dynamics, (ii) exploring response amplitudes and motion trajectories as a function of flow and structural parameters, and (iii) gaining insights into the vortical structures of the flexible cantilever during sustained oscillations. The results of the numerical simulations reveal that within a specific range of the reduced velocity parameter (U*), the cantilever undergoes sustained oscillations. A characteristic tip motion trajectory resembling a figure-eight shape is observed during the beam’s oscillatory behavior.

In addition to full-order simulations, a novel application of a graph neural network reduced order model (GNN-ROM) is explored to serve as a surrogate model for the flexible cantilever problem. The integration of GNN-ROMs aims to enhance predictive capabilities by leveraging graph-based representations of the fluid-structure system. The utilized model integrates the quasi-monolithic graph neural network outlined in Ref. [3]. Operating within the ALE framework, the model employs a multi-layer perceptron for the evolution of mesh displacements and a hypergraph neural network to forecast fluid states based on the present system state. The structural state is implicitly represented through the dynamic movement of the mesh at the fluid-structure interface. Using the full-order numerical simulation data, the model is being trained and validated for various fluid-structure conditions.

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Machine learning for design tasks and inverse problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MATERIAL-MODEL CALIBRATION FOR DUCTILE METALS USING RADIOGRAPHS OF HIGH-EXPLOSIVE DRIVEN EXPERIMENTS

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ABSTRACT

We present an application of convolutional neural networks to calibration of material-physics models from radiographs of high-explosive induced shock experiments. Material properties for metals and polymers undergoing explosive loading are often poorly understood and are calibrated under simplified experimental conditions, for example uniaxial shock compression, where good physical models of the process exist. For more complex two- and three-dimensional loading regimes velocimetry gives an incomplete picture of the process and dynamic radiographs are used to understand the material properties. Unfortunately, directly relating features of a radiographic image to a material-model calibration is often intractable and the analysis of radiographs becomes necessarily qualitative. With simulation-informed neural-learning we can develop a more quantitative analysis. In this work we use a high-fidelity, multi-physics simulation developed at Los Alamos National Laboratory, to simulate hundreds of variations of a high-explosive shock experiment. The variations are chosen to span the uncertainty in the material-physics process of interest as well as uncertainty coming from experiment timing and secondary materials involved in the experiment. For each simulation we produce a suite of synthetic radiographs that captures uncertainties of the radiographic observation process. From this synthetic radiograph data we train neural networks to learn the inverse mapping between radiograph and material parameters. It is demonstrated that, using a simple convolutional architecture, trained networks can infer material calibrations from synthetic radiographs with high accuracy. Moreover, by using Bayesian-network approaches we can produce estimates of material calibrations with quantified uncertainty. Physics applications of machine-learning methods must be accompanied by an analysis of how networks are making their inferences to build confidence in these predictions and to predict likely shortcomings in the technique. Leveraging a particular network structure, we are able to examine learned-features our model extracts by looking at individual layer outputs. It is shown that our networks heavily weight physically-defensible features in the image during regression. In this talk we give a detailed description of our data-generation methods and the learning problems we address. We then outline our neural architecture and training approach. Methods for human interpretation of the network's inference process are put forward, including techniques to assess sensitivity of inferences to learned features.

Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SEMI-IMPLICIT MATERIAL POINT METHOD FOR UNSATURATED SOIL WITH CONSTITUTIVE MODEL DEPENDING SUCTION

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ABSTRACT

Hazardous landslides caused by heavy rainfall. In this situation, the slopes lose the suction, which is the shear resistance of soil, by transitioning from unsaturated to saturated states. To simulate this process, particle-based methods have become popular, and among them, the material point method (MPM) has accomplished a remarkable progress in the area of computational geomechanics.

The MPM is a particle method, but the algorithm is similar to the finite element method (FEM) and uses an Eulerian mesh to solve a set of governing equations. Thus, comparing with other particle methods, the MPM does not require searching for neighbor particles, and this advantage reduces the computational cost. Nevertheless, most of the previous MPM developments for unsaturated soil suffer from two demerits, when explicit time integration is adopted. One is the pore water pressure oscillation caused by using the large water bulk modulus, and the other is the large computational cost. Alternatively, semi-implicit MPMs equipped with the so-called fractional-step method have been proposed by several scholars [1] to overcome these problems. However, few studies have so far been made to deal with large deformation of slopes made of unsaturated soil.

To address this problem, we have recently developed the semi-implicit MPM for unsaturated soil based on Biot’s mixture theory [2]. However, in the simulation of the model experiment, which is infiltration-induced sand slope failure, there is a slight discrepancy between the analysis and experiment results in the timing and mode of failure. This is due to the local reduction of the cohesion and the internal friction angle with respect to the suction as the water seepage. Thus, to improve the performance of failure simulation, we incorporate the suction effect to the cohesion and the internal friction angle in the constitutive model, which is the Hency's hyperelastic model with the Drucker-Prager model. Several numerical examples are presented to demonstrate the capability and performance of the semi-implicit MPM with presented constitutive model. In particular, to validate it with respect to the suction, the analysis is carried out for simulating a model experiment of infiltration-induced failure.

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Computational methods in environmental fluid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTIPLE TIME SCALES AND VARIABLE BOTTOM TOPOGRAPHY FOR DISCONTINUOUS GALERKIN LAYERED OCEAN MODELING

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ABSTRACT

In the numerical modeling of ocean circulation, it is a widespread practice to employ a barotropic-baroclinic time splitting, for which the fast external motions are modeled by a vertically-integrated (barotropic) system that is similar to the shallow water equations and is solved with a relatively short time step. The remaining motions are modeled by solving the full dynamical equations in each fluid layer with a relatively long time step; the present talk is concerned with layered (isopycnic) models, for which the vertical coordinate is a quantity related to density. A barotropic-baroclinic time splitting raises issues that include the following: (1) There needs to be suitable communication between the two subsystems. (2) The layer equations include motions that vary on the fast time scale, so the algorithm must include a mechanism that enables stability when the long time step is used. If a layer interface intersects variable bottom topography, some additional issues include the following: (3) In this case a physical layer thickness can tend to zero, and a numerical approximation to this thickness must remain nonnegative. (4) If sufficient care is not taken, the extracted velocities can be erratic and cause CFL violations. Various steps must be taken to address the above issues. The present talk will describe one of these steps, in which the issues (1)-(2) are closely related to (3)-(4), for the case where a discontinuous Galerkin method is used for the spatial discretization.

Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A DEEP-LEARNING BASED SURROGATE MODEL FOR SHELL HOMOGENISATION: APPLICATION TO THE FAILURE ANALYSIS OF LAMINATED COMPOSITES

Aewis KW Hii[*1], Bassam El Said[1] and Stephen R. Hallett[1]*

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ABSTRACT

In this work, we present a data-driven multi-scale analysis framework for shear-deformable shell finite elements, with application to the progressive failure analysis of laminated composite structures. The framework formulation is rooted in second-order homogenisation [1], with which we have expanded on [2] to allow for the homogenisation of thick shells. When used in a concurrent FE2 analysis, the model yields an accurate estimation of the transverse shear stresses in thick shell problems. As a result, this allows the multi-scale shell element to accurately model in-plane damage and delamination as degradations in the shell stiffness. However, a concurrent framework consumes excessive computational resources and does not scale up for application to large components. To overcome this, we are using a deep learning based surrogate model in place of the online RVE analysis.

The novel contribution here is the creation of a surrogate for the constitutive responses of shells, with application to the failure analysis of composite structures. Unlike their solid counterparts, additional deformation modes such as bending, twisting and higher-order transverse shear need to be considered in shells. These factors significantly increase the dimensionality of the input and output space. In addition, shell homogenisation incorporates length-scale information such as thickness and local shell curvature, and the RVE size approaches that of the structural component. As a result, the combinations of strains seen by a shell element can vary substantially across different clusters of structural geometry and loading/boundary conditions. Therefore, here, we are also augmenting the surrogate model's input space so that the shell material model can generalise to unseen cases.

In summary, this work features a multi-scale shell analysis framework that can predict progressive 3D damage in composite structures, and it builds on existing techniques from second-order homogenisation and deep learning. The long-term objective is to build a fast and robust framework to model complex materials at the structural length scale, which will aid in design space exploration and part optimisation.

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Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPLICIT MESHFREE METHODS FOR PREDICTIVE SOLUTIONS IN EXTREME MECHANICS

Michael Hillman[*1], Joseph Magallanes[1] and Dominic Wilmes[1]*

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ABSTRACT

In this talk, I will give a general overview of meshfree techniques used in high-strain-rate simulations. The critical aspects of variational consistency (passing the patch test) and convergence, spatial stability of the node-based equations (kernel, tension, and rank stability), and representation of material stability and instability will then be discussed. Following [1-4] I will show that unless special care is taken, these properties are not guaranteed. For instance, passing the patch tests is non-trivial for most meshfree methods, and proper representation of material stability is generally not obtained without strain-smoothing techniques. It is then shown that the reproducing kernel particle method with natural strain-smoothing stabilization is among the few methods that possess all these essential properties. Results are presented for challenging applications such as fragment-impact problems.

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SPLINE-BASED PARAMETERISATION TECHNIQUES FOR PLANE GRAPHS

Jochen Hinz[*1] and Annalisa Buffa*[1]

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ABSTRACT

Isogeometric Analysis (IGA) has emerged as a promising variant of classical FEM for modeling complex problems arising in real-world physical systems. Unlike FEM, IGA employs the de-facto CAD standard of spline-based parametric descriptions for representing the geometry. The same spline technology is then employed as a basis for analysis. Despite the promise of mitigating the CAD to FEM geometrical conversion overhead, Isogeometric Analysis (IGA) has witnessed the development of innovative numerical schemes that leverage the advanced smoothness inherent in spline basis functions. A common challenge in engineering applications is generating a conforming parameterisation of a domain composed of several faces, where only the descriptions of the faces' boundaries are available. In this setting, the geometry can be represented as a plane graph composed of vertices and edges, wherein each edge represents a spline curve or a dense point set. These edges are organized into groups that form closed loops, each representing the boundary of a face.

The purpose of this talk is presenting spline-based parameterisation techniques for plane graphs, respecting the requirement that each face be parameterised individually to, for instance, impose locally differing material parameters. We adopt the concept of harmonic maps as the underlying parameterisation method which is then applied to the faces one-by-one. Each face's multipatch layout is selected from a large catalogue of multipatch templates. The presented technique produces a multipatch paramterisation with a conforming interface between the faces while offering a large degree of automation. It may then be utilized for numerical simulation based on IGA, or converted back into an arbitrarily-dense classical mesh by collocating the face's surface splines.

PSE (Problem Solving Environment)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT OF NET MORAL EDUCATIONAL MATERIALS TO PROTECT YOUTH FROM HARMFUL ENVIRONMENTS

*Shinji Hioki**[1]

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ABSTRACT

In recent years in Japan, the number of young people who are exposed to the Internet has been increasing due to the younger age of Internet users and the spread of smartphones and tablets, and the number of young people who are victims of Internet crimes has been increasing. The number has increased approximately 1.3 times in the past 10 years. Various countermeasures are being considered, and as one of them, educational materials on net morals are being developed. The current situation will be reported.

Fluid-structure interaction: Methods and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ASSUMPTION BULGING FREQUENCY OF THE REAL SCALE TANK BY MICRO-TREMOR MEASUREMENT AND THE EIGENVALUE ANALYSIS

Shu Hirai[*1], Taisuke Ono[2], Hirokazu Hirano[1] and Naotsugu Sato[1]*

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ABSTRACT

In Japan, there have been numerous reports of damage caused by the expansion of water storage tanks during earthquakes which are seismic intensity of 6 or higher, including the 2011 Great East Japan Earthquake and the 2016 Kumamoto Earthquake1). Bulging2) refers to the coupled vibration between tank wall and content fluid. This phenomenon is induced by seismic ground motion. In Japan, seismic design against bulging is introduced quite recently in 2022, which will activate various kind of engineers' interests on it.

Therefore, existing water storage tanks should be promptly examined to determine whether or not bulging will occur and, the method for judgement is required. For this purpose, it is important to understand the natural frequencies of the side walls of the tanks.

In this study, micro-tremor measurement and the eigenvalue analysis to calculate the natural frequency are conducted to estimate the natural frequency. According to the hypothesis of this paper, the real scale stainless panel tanks have natural frequency below 10 Hz, at which bulging damage occurs. According to Ochiai's research3), the frequency of earthquake in nature is roughly 10 Hz or lower, and even when it is higher, the energy of the earthquake is small. In the measurement, the micro-tremor measurement device is installed on the ceiling of the tank and vibrations are measured after lightly tapping on the side walls, followed by spectral analysis and comparison with the results of natural frequency analysis.

As a result, the calculated natural frequency of bulging is consistent with that of the real scale tank, indicating the possibility of bulging occurring in the tank. We found that the micro-tremor measurement method is particularly effective for stainless steel panel tanks, which are considered to have natural frequencies below 10 Hz or less.

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Recent advances in meshfree and particle methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FLUID FILM LUBRICATION SIMULATION OF PRESSURE-DEPENDENT NON-NEWTONIAN FLUID USING THE MOVING PARTICLE HYDRODYNAMICS METHOD

Shu Hiramoto[*1], Kazuya Shibata[1], Kyuya Matsumoto[1], Hideyo Negishi[2] and Masahiro Kondo[3]*

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ABSTRACT

When a fluid is subjected to extremely high pressure, its viscosity can increase dramatically because the distance between molecules decreases and the intermolecular force increases. Such pressure-dependent non-Newtonian fluid phenomena occur in fluid film lubrication [1] and are difficult to simulate using traditional particle methods. This is because in fluid film lubrication, the lubricant flows in an extremely narrow gap and the fluid pressure fluctuates due to the significant change in viscosity.

In this study, we developed a new model for non-Newtonian fluids whose viscosity changes significantly with pressure. The present model is based on the moving particle hydrodynamics (MPH) method [2] and Roelands' viscosity-pressure equation [3]. The MPH method is characterized by its discrete dynamic stability, which is ensured by the theory of analytical mechanics. Isothermal fluid film lubrication in line contact was simulated in two dimensions with the present model, and the simulated pressure distribution was compared with the numerical solution of the conventional Reynolds equation.

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Multiscale modeling, analysis and numerical methods of material defect and inhomogeneities
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ENABLING LOCAL LATTICE STRUCTURE ANALYSIS IN FINITE TEMPERATURE MOLECULAR DYNAMICS SIMULATIONS

Atsuo Hirano[*1] and Akiyuki Takahashi*[1]

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ABSTRACT

Molecular Dynamics (MD) has been widely used to calculate material properties and simulate deformations and fractures of materials with atomic scale. To reproduce experimental results, it is inevitable to perform MD simulations at high temperatures and analyze the local lattice structures. However, it is difficult to analyze the local lattice structures in MD simulations at high temperatures because of the atomic thermal fluctuations. Up till now, various methods are used to solve the problem. To minimize the atomic thermal fluctuation, the simulations were performed at only lower temperatures [1]. However, with the method, it is impossible to reproduce the phenomena peculiar to the high temperatures. Others used the structure relaxation methods at every simulation time step [2][3] although the methods need extensive computational costs. Therefore, it is desired to have a computationally efficient numerical method to enable the accurate local lattice structure analysis in MD simulations even at high temperatures.

This paper presents a new method to reduce atomic thermal fluctuation with a simple algorithm to enable us to identify local lattice structures accurately even at high temperatures. In the method, we introduce new degrees of freedom called "Markers" which are connected to atoms. Since the thermal fluctuation of Markers is reduced, the local lattice structure analysis can be performed accurately with the reduced thermal fluctuations using Markers. The computational cost of Markers is very low, and only one parameter is added for our method.

We verified the performance of this method. The error rate of the structure identification using common neighbor analysis (CNA) can be almost 0% under 1200 K in Fe with our method whereas it becomes about 5% without it. Moreover, the average distance between atoms and Markers can be under 0.1 Å. Therefore, our method can have a good performance of both the thermal fluctuation reduction and the trackability to atoms. Subsequently, our method was applied to the phase transformations in Fe at high temperatures. We observed clearly the phase transformation from face centered cubic (FCC) structure to body centered cubic (BCC) structure. It is expected that our method can be applied to various simulations at high temperatures.

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Extended digital twins including uncertainty and complexity of human/society and human knowledge
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INTEGRATING HUMAN UNCERTAINTY AND CREATIVITY INTO THE EXTENDED DIGITAL TWIN: KNOWLEDGE IS ALL YOU NEED

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ABSTRACT

To further develop Society5.0, which advocates human-centered CPSs (Cyber-Physical Systems), and to realize a new paradigm of Japanese manufacturing and social eco-system, we first classify the factors of uncertainty and complexity in the CPS process into uncertainty related to things and uncertainty related to events. Uncertainty related to things can be defined from a quality engineering perspective as factors such as uncertainty related to data and measurements from products (devices) in usage conditions, and variations in boundary conditions and material properties related to models on the Digital Twins. On the other hand, uncertainty related to events is defined to include more complex and unstable ones due to the dynamic changes caused by the complex and uncertain human/social systems.

Then, we define Extended Digital Twins as Digital Twins including the uncertainty and complexity inherent in humans and society. Several mathematical models for human characteristics including emotion, bounded rationality, and creativity are considered. The acquisition and generation of related knowledge from various perspectives are also investigated. The extraction processes of experiential and tacit knowledge of humans in product planning, design, and development, and even in the areas of production, logistics, supply chain, sales, and service operations, are pursued by generative AI. In particular, human emotions are evaluated based on the free-energy principle, and human creativity is considered based on normalized entropy.

Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMPACT FRACTURE ANALYSIS METHOD AND ITS APPLICATIONS TO EDGE CHIPPING OF GLASS

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ABSTRACT

The impact fracture problem entails dynamic loading accompanieded by stress wave propagation and energy dissipation during collision. Due to these conditions, simulating fracture under dynamic loading is significantly more challenging than under quasi-static loading. In this research, we enhance Particle Discretization Scheme Finite Element Method (PDS-FEM), developed by the authors, to simulate fracture and collision of two objects simultaneously. Subsequently, we apply the proposed method to the simulation of edge chipping of glass.

Edge chipping is caused by concentrated loading applied near a sharp edge of brittle materials. This type of fracture results in the removal of a conchoidal chip from materials and is commonly observed during the manufacturing process. We conducted numerical analyses on the edge chipping of soda-lime glass, subjecting it to the impact of a rigid steel sphere while varying the size of the sphere, impact velocity, and impact distance from the glass edge. Our numerical analysis successfully reproduces 3D complex crack patterns, including Hertzian cone cracks and conchoidal chip scars. To the best of our knowledge, this is the first detailed simulation of the 3D crack morphology in edge chipping. We anticipate that our numerical analysis method is widely applicable to impact fracture studies.

Innovations in machine learning-enhanced uncertainty quantification for computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMPLEMENTING UNCERTAINTY QUANTIFICATION CALIBRATION WHEN PREDICTING FALL PARAMETERS OF IMPACT-INDUCED SKULL FRACTURES IN INFANTS

Jacob Hirst[*1], Brian Phung[1], Bjorn Johnsson[1], Brittany Coats[1] and Ashley Spear[1]*

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ABSTRACT

In 2021, 7.1 million children were victims of child abuse [1], with infants < 1 year of age at the greatest risk of injury and death from abusive head trauma. Infants cannot communicate instances of abuse; thus, verifying reported histories of head trauma (accident versus abuse) is a critical and challenging task for child advocates in the early detection of child abuse. Physics-based models of infant skull fracture can provide valuable insight into patterns that could distinguish between accidental and abusive trauma. Previously, we developed a numerical framework to predict fracture patterns in infant skulls [2]. Using the framework, fall scenarios can be simulated to predict skull fracture to corroborate or refute witness statements in cases of suspected abuse, but the computational expense of these simulations is high and requires considerable specialized effort. To overcome this challenge, several machine learning (ML) models were trained on a finite number of fall simulations to predict fall parameter probabilities given specific skull fracture features extracted from the simulations. The ML models included a random forest (RF) regressor, a Gaussian process regressor (GPR), an artificial neural network (ANN), polynomial regression, ridge regression, lasso regression, and linear regression models. To account for model inaccuracies, bagging ensemble UQ strategies were used with ensembles of the ANN, GPR, and RF and compared to the inherent UQ abilities of the RF and GPR. We then employed a UQ calibration technique that uses linear and exponential scaling on the uncertainty [3]. The calibration method is used on each of the original strategies of UQ, and the uncalibrated uncertainties are compared with the calibrated uncertainties. Quality of uncertainty was measured with plots of residuals vs predicted uncertainty, where the slope of these plots would ideally be 1, and the intercept 0. The calibration method resulted in improved average slopes on test sets across a 5-fold cross-validation. These results suggest that calibration techniques refine the accuracy of UQ for these strategies which, in turn, refine the ML tools mentioned. This results in a more reliable prediction of fall parameters associated with skull fracture patterns, potentially adding a valuable tool for medicolegal teams to use when differentiating an accident from abuse.

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Next-generation numerical methods for coupled multiphysics problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LOCAL TIME-STEPPING DECOUPLED ALGORITHMS FOR FLOW AND TRANSPORT PROBLEMS IN FRACTURED POROUS MEDIA

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ABSTRACT

The numerical simulation of flow and transport in a porous medium with fractures is challenging due to the presence of multiple spatial and temporal scales and strong heterogeneity of the domain of calculation. A fracture may have much higher or much lower permeability than that in the surrounding medium, thus the time scales in the fractures and in the rock matrix may vary significantly. In addition, the width of the fracture is much smaller than any reasonable parameter of spatial discretization. To tackle those challenges, we first consider a dimensionally reduced fracture model, where the fracture is treated as a hypersurface embedded in the porous medium. Then we develop domain decomposition (DD) methods that allow the use of different time step sizes in the subdomains and in the fracture. For each DD method, a space-time interface problem is formulated, based on either the physical or optimized transmission conditions imposed on the fracture-interface. Such an interface problem is solved iteratively and globally in time. The proposed methods are fully implicit and are designed to converge fast while preserving the accuracy in time with nonconforming time grids. Convergence analysis as well as numerical results will be presented for the flow problem of a single phase, compressible fluid, and the linear advection-diffusion equation with high Péclet numbers.

Computational fluid dynamics (CFD) and fluid-structure interaction (CFSI): Methods and Applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HYDROELASTIC VIBRATIONS OF PRESTRESSED ELASTIC TANKS COMPUTED WITH ISOGEOMETRIC ANALYSES AND PROJECTION BASED REDUCED ORDER MODEL

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ABSTRACT

The goal of this study is to use Isogeometric Analyses (IGA) [1] for the computation of coupled fluid-structure vibrations with prestressing effects. This topic is relevant in the context of aerospace applications for the design of pressurized liquid launcher propellant tanks. The major objective is to estimate numerically, with IGA, the prestressed hydroelastic vibrations, defined as the coupled vibrations of an elastic structure around a geometrical nonlinear equilibrium in contact with an incompressible free-surface liquid.

The use of the IGA framework, which conserves the geometry from computer aided design models, provide robust frequency estimations in linear structural vibrations [1]. Recent studies have been carried out with IGA for linear hydroelastic vibrations of partially filled structures without prestressed effects showing good agreements between numerical and experimental studies [2]. In the present study, comparisons between Finite Element Method (FEM) and IGA are expected, particularly for 3D geometries using a Projection Based Reduced Order Model (PROM) framework [3]. The methodology is the following. At first, a reference solution using FEM without PROM will be provided to compute the hydroelastic modes for a 3D fluid-structure problem. Comparison using IGA will be proposed with and without PROM procedures.

Errors and convergence rate will be presented to demonstrate the effectiveness of this methodology in the context of prestressed hydroelastic vibrations with PROM using IGA or FEM.

Key Words: Hydroelasticity, Isogeometric Analysis, Projection Based Reduced Order Model

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Advances in damage & fracture modeling of multiphysics materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NESTED PHFGMC MICROMECHANICAL MODELS FOR THE NONLINEAR AND DAMAGE OF AUTOMATED FIBER PLACEMENT COMPOSITES

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ABSTRACT

Automated Fiber Placement (AFP) is an advanced composite manufacturing technology widely used in the aerospace and automotive industries. The AFP technology offers advantages such as improved production efficiency, reduced material waste, and the ability to create complex geometries that may be challenging with traditional manufacturing methods. However, one critical challenge yet to be thoroughly investigated in AFP-composites is predicting elastic properties and damage that may arise from a wide range of inconsistent material properties compared to composites manufactured using traditional technologies. An important aspect is the effect of inherent gaps between material tows and fiber misplacement during the AFP process. To that end, the Parametric High-Fidelity Method Generalized of Cells (PHFGMC) micromechanical mode is employed to construct hierarchical nested models of AFP-composites at the micro and meso levels. The PHFGMC has been established as an advanced micromechanical approach well-suited for analyzing the nonlinear behavior of diverse periodic composite materials. The PHFGMC is a refined dedicated micromechanical model capable of accurately predicting the local-global responses of heterogeneous multiphase composites. In the PHFGMC method, periodicity conditions are imposed between the boundaries of a repeating unit cell (RUC). The RUC can be divided into general quadratic or hexahedral subcells representing the different phases. Average traction and displacement continuities are enforced between the subcells to achieve equilibrium requirements between the adjacent subcells. In addition, a new formulation based on average virtual work was recently introduced for the PHFGMC. This approach is suitable for micromechanical calculations and has comparable computational efficiency to the finite element method [1, 2].
The proposed research investigates nested micromechanical AFP carbon/epoxy material systems models. Therefore, the PHFGMC-RUC is constructed using micrographs to capture the AFP microstructure. Further, results are compared to experimental data to demonstrate the ability of the new PHFGMC-AFP to predict a wide range of mechanical properties.

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Numerical methods, mathematical modeling and analysis in material science
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AUTOMATED AB INITIO-ACCURATE ATOMISTIC SIMULATIONS OF DISLOCATIONS

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ABSTRACT

A well-known drawback of state-of-the-art machine-learning interatomic potentials is their poor ability to extrapolate beyond the training domain. For small-scale problems with tens to hundreds of atoms this can be solved by using active learning which is able to select atomic configurations on which a potential attempts extrapolation and add them to the ab initio-computed training set. In this sense an active learning algorithm can be viewed as an on-the-fly interpolation of an ab initio model. For large-scale problems, possibly involving tens of thousands of atoms, this is not feasible because one cannot afford even a single density functional theory (DFT) computation with such a large number of atoms.

In this talk, I will present an active learning algorithm for simulating dislocations that identifies local subregions of the simulation region where the potential extrapolates [1,2]. Then the algorithm constructs periodic configurations out of these local, non-periodic subregions, sufficiently small to be computable with plane-wave DFT codes, in order to obtain accurate ab initio energies. The algorithm is tested on two relevant types of dislocations, screw dislocations in bcc tungsten, and dissociated dislocations in fcc aluminum, and I will show that our algorithm reaches near-ab initio accuracy for material properties such as core structure, Peierls barrier, and Peierls stress.

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Multiphysics and data-driven modeling for cardiovascular biomedicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTATIONAL ANALYSIS OF TURBULENT FLOW STRUCTURES IN THE LEFT VENTRICLE OF THE HEART USING PATIENT-SPECIFIC DATA

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ABSTRACT

Blood flow in the left ventricle is characterized by the change in ventricle volume over the heart cycle, the structure of the inner ventricular wall, blood characteristics, and the associated inflow and outflow regulated by the mitral and aortic valves, respectively. In systole the ventricle contracts which leads to an increase in blood pressure, which in a healthy heart closes the mitral valve to the left atrium and opens the aortic valve for the blood to flow into the aorta. Analogously, in diastole, the heart relaxation phase, the ventricle expands, blood pressure drops, the aortic valve is closed and the mitral valve opens to let blood flow into the ventricle from the left atrium. The inflow in diastole has two phases, the E-wave followed by the A-wave, each representing jet flow which breaks down into turbulent flow in the ventricle. Heart valve disease may lead to restricted valve openings, or leaking valves, that changes the blood flow in the ventricle. Similarly, clinical interventions may lead to changes in the ventricular blood flow.

Blood cells and endocardial cells respond to mechanical stresses in the blood flow, and changes in the mechanical stresses may be a risk factor e.g. for thrombosis. In this work we use patient-specific data to build a computational model of the blood flow in the left ventricle of the heart, in which we analyse the mechanical stresses in the blood flow, with a focus on the turbulent flow structures in diastole. The computational model is based on solving the Navier-Stokes equations with a finite element method on a deforming mesh, and the mechanical stresses are analyzed using the triple decomposition of the velocity gradient of the flow.

In previous work we have established a clinical pathway for patient-specific simulations through which we analyzed turbulent flow structures in a finite element model where the mitral valve was modelled as a time varying inflow boundary condition [1]. We here extend this framework to a more realistic simulation using a fluid-structure interaction model of the mitral valve based a unified continuum approach [2].

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Advanced materials: Computational analysis of properties and performance
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTATIONAL MODELING OF FIBER-REINFORCED COMPOSITE LAMINATES UNDER HIGH-CYCLE FATIGUE LOADING

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ABSTRACT

Fatigue is an important failure process and is often governing for the design of fiber reinforced polymer composites. In recent years, significant progress has been made in accurately simulating high-cycle fatigue crack propagation in composite specimens with initial cracks. However, numerical methods for simulating the complete progressive failure process in laminates are far less matured. In multidirectional laminates, delamination, transverse matrix cracking and ultimately fiber breakage can occur in distinct plies. Virtually testing these complex laminates requires progressive failure modeling frameworks capable of capturing all relevant failure processes and their interaction. Moreover, these frameworks must not only consider propagation of transverse matrix cracks and delamination, but also the initiation of cracks in pristine material.

In this contribution, we present an accurate, efficient and robust progressive failure framework for simulating the interaction between several failure processes under high-cycle fatigue loading. A mixed-mode fatigue cohesive zone model [1], covering both initiation and propagation of fatigue cracks, is embedded in a mesoscale framework [2] for describing the traction-separation relation of inter- and intra-laminar fatigue cracks. The cohesive zone model is based on S-N curves and requires only a few material parameters related to fatigue damage, without using Paris data as input for describing propagation of fatigue cracks. Furthermore, XFEM is used to allow for discrete intra-laminar cracks at arbitrary locations. Discontinuities, representing transverse matrix cracks, are inserted in the elements as soon as a proper fatigue crack insertion criterion is reached. With this approach, a transition from distributed cracking to localized failure can be simulated. Moreover, the effect of thermal residual stresses due to the curing process is taken into account in an adaptive cycle jumping scheme where explicit sinusoidal load cycles are applied before a jump in cycles takes place. With this scheme, the local stress ratio, which varies in the laminate due to non-uniform residual stresses, can be determined in each material point and subsequently used in the (local) constitutive model for the calculation of fatigue damage.

It is shown through numerical examples of open-hole laminates with complex failure mechanisms that the modeling framework is capable of accurately capturing initiation, propagation and interaction of intra- and inter-laminar failure processes. Furthermore, the model shows a good match in fatigue life and damage evolution when compared against experimentally tested quasi-isotropic open-hole laminates.

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SciML in the real world
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ACTIVE LEARNING METHODS FOR TRAINING FREE ENERGY MODELS

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ABSTRACT

We have developed active learning methods to improve data sampling and training for problems in materials physics. Included among these are inverse problem wherein the goal is to determine material properties or mechanisms based on computational and/or experimental data. In the context of initial and boundary value problems, there are often locations in the domain which require dense sampling due to the complexity of the region. However, there are often constraints with our ability to sample data densely over the whole domain. Active learning methods enable us to query data where it will be most useful to ensure a well trained model. We have shown the effectiveness of applying active learning methods to a scale bridging process which uses first principles and statistical mechanics data to determine a free energy surrogate model [GH Teichert, S Das, M Faghih Shojaei, J Holber, T Mueller, L Hung, V Gavini, and K Garikipati. Bridging scales with machine learning: From first principles statistical mechanics to continuum phase field computations to study order disorder transitions in lixcoo2. arXiv preprint arXiv:2302.08991, 2023]. The active learning methods enable us to intelligently sample in a high-dimensional space, allowing us model details related to ordering in our phase field simulations, that are not generally available. We have continued to develop additional active learning methods for adaptative sampling and model parameters and training. The adaptive sampling methods include sampling in regions of interest: wells, non-convexities, etc and sampling in regions of high error, data sensitivity, and data variability. These methods enable the creation of free energy models which provide additional insight into materials using fewer data points.

Constitutive modeling of complex materials with machine learning and artificial intelligence
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICS-INFORMED CRYSTAL PLASTICITY RNN FOR TEMPERATURE-DEPENDENT ANISOTROPIC PLASTICITY IN HCP MATERIALS

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ABSTRACT

Neural network surrogate models for constitutive models in computational mechanics have been developed and employed for a while. Especially in the field of plasticity, these models are often developed on the basis of existing GRU or LSTM cells that have a proven capability to learn path-dependent phenomena. Major drawbacks of these architectures, however, include the relatively long training times and a time-resolution dependent prediction that extrapolates poorly. Further, most existing work for macro- or mesoscopic surrogate models in plasticity is content to predict relatively simple material behaviors. Hence, in this work, the focus lies on circumventing these drawbacks. We formulate a time-resolution independent neural architecture on the basis of the recurrent neural operator and apply it to learn the temperature-dependent plastic response of magnesium, known for its pronounced plastic anisotropy and thermal dependence. The recurrent neural operator predicts the material behavior withgreat accuracy and is shown to generalize well for various loading cases and temperatures, as well as time-resolutions. Furthermore, it clearly outperforms existing GRU and LSTM models in terms of training and predictive performance. Finally, we perform multiscale simulations with the RNO and achieve at least three orders of magnitude speed-up compared with existing physical models.

Constitutive modeling of complex materials with machine learning and artificial intelligence
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

QUANTIFYING MODEL-FORM UNCERTAINTY IN CONSTITUTIVE MODELING: A PHYSICS-INFORMED INFORMATION FIELD THEORY APPROACH

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ABSTRACT

Uncertainty quantification (UQ) is often critical for physical inverse problems (inferring a physical model from data). This is especially true when data are sparse or noisy. When solving inverse problems, it is common practice to fix a form for the physical model (e.g., which terms show up in the differential equation) and only then find the probability of the model parameters. However, this approach underestimates uncertainty because it assumes reality can be fully captured by the chosen model form. Physics-informed Information Field Theory (PIFT) is a new, fully-Bayesian framework which quantifies uncertainties coming from the lack of knowledge of the model form (as well as from lack of knowledge of model parameters and from measurement error). PIFT differs from many other model-form UQ methods in that one does not need a library of potential models. Instead, one constructs a prior probability distribution over the function space of all possible physical models. This distribution assigns higher probability to models which obey the hypothesized physics (e.g., a particular constitutive model), with a parameter controlling the degree of trust in the hypothesized physics. We demonstrate the PIFT framework with examples in constitutive modeling and show how it can also deal with ill-posed problems.

AUTOMATED MODEL DISCOVERY USING INELASTIC CONSTITUTIVE ARTIFICIAL NEURAL NETWORKS (ICANNS)

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ABSTRACT

For solids, centuries of research in the field of physics and mechanics have guided us towards the uncertainty-free conversational laws in continuum mechanics. Following these principles of thermodynamics, material models have been derived that obey these laws. Unfortunately, certain models are only able to explain a specific material behavior. In practice, we usually pre-select a particular model and try to find the best material parameters corresponding to that model to fit our data; instead, it is our strong belief that we should find the best model explaining our data. This is where machine learning algorithms help us achieve this paradigm shift. Since these algorithms lack from knowledge of thermodynamics, it is not surprising that they learn the data used for training very well, but their ability to predict material behavior outside the training regime is disastrous and, most of the time, unphysical. This is already the case for elastic materials and is even worse for inelastic material behavior. To overcome this issue, a family of Constitutive Artificial Neural Networks [1] has been developed that combines thermodynamic knowledge with modern machine learning techniques. These networks are designed for elastic material behaviour and satisfy thermodynamics a priori. As most materials exhibit inelastic deformations, a critical missing link is to expand the general concept to inelastic materials. One way to do so is to introduce a pseudo potential depending on stress-like quantities associated with the inelastic rate [2]. Here we extend CANNs to inelastic material behavior (iCANN) [3]. Therefore, our network discovers both the Helmholtz free energy and the pseudo potential, which explain the experimental data the best. As the design is not limited to a specific inelastic phenomenon, thermodynamics are satisfied a priori regardless of the inelastic behavior. Our vision for iCANNs is that they help us to reveal the various inelastic phenomena hidden in the data, such as plasticity, viscosity, phase transformation, degradation, growth and remodeling. For illustrative purposes, we specialize the general architecture of our iCANN to visco-elasticity and demonstrate that it is capable of discovering a model for polymers and skeletal muscle data.

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Multi-physics and multi-scale simulations with the coupling library preCICE
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A COUPLED TWO-MUSCLE-ONE-TENDON MODEL OF THE AGONIST-ANTAGONIST MYONEURAL INTERFACE

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ABSTRACT

Conventional amputations destroy the mechanical link between the agonist-antagonist muscle pair. A novel surgical approach, the agonist-antagonist myoneural interface (AMI), aims to mitigate the amputation's damage by surgically re-connecting the naturally paired muscles with a tendon, so that the mechanical and sensory connection is maintained.

Skeletal muscles are made of an active hierarchical tissue, with each muscle containing thousands of muscle fibers and millions of sarcomeres, the smallest contracting unit. We model skeletal muscles with OpenDiHu, an HPC framework for neuromuscular simulations that couples a 3D finite element mechanics muscle to a model for the action-potential propagation through 1D muscle fibers and a model for the electro-chemical phenomena in the sarcomeres. OpenDiHu is capable of mapping between meshes and time subcycling, so that all models are embedded in a single OpenDiHu muscle solver.

We use this muscle solver to develop a two-muscle-one-tendon AMI model using preCICE. The agonist and the antagonist muscles are modeled by identical OpenDiHu solvers, while the tendon participant is modeled by a simpler, 3D finite element OpenDiHu solver.

We model the mechanical coupling of the muscles through the tendon using the fully-implicit multi-coupling scheme in preCICE. In each coupling iteration, values of displacement, velocity and traction are exchanged across adjacent surfaces. Results show that when one muscle contracts, the tendon is displaced and the other muscle elongates as expected.

We aim to involve neural coupling as well, so that we can model the monosynaptic and disynaptic reflexes, i.e., the exchange of proprioceptive information. Thereby, we expand our muscle solver with models of sensory organs, e.g., muscle spindles and the motor neurons that activate muscle fibers. Our plan is to connect the agonist-antagonist muscles directly using two additional serial-explicit schemes to account for the reflex feedback loops and combine them with the multi-coupling scheme for mechanical coupling. As a result, challenging circular loops for communication arise.
We are making steps towards the integration of neural coupling in our two-muscle-one-tendon model, and all the different required OpenDiHu models already exist independently. We are also working to use real muscle geometries obtained from patient imaging. In the long run, we intend that our two-muscle-one-tendon AMI model is used as a tool for surgeons to decide on critical anatomical parameters, such as the prestretch of the muscles, prior to the AMI procedure.

Quantum scientific computing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT OF AN INFINITESIMAL DEFORMATION ANALYSIS METHOD FOR TRUSS STRUCTURES BASED ON A QUANTUM APPROXIMATION OPTIMIZATION ALGORITHM

Rio Honda[*1], Katsuhiro Endo[2] and Mayu Muramatsu[1]*

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ABSTRACT

In this study, we develop a deformation analysis method for truss structures using the Quantum Approximate Optimization Algorithm (QAOA) [1]. Structural analysis is crucial in the field of engineering to evaluate the durability of structures and to derive optimal structures. However, as the size of the structures under analysis increases, the computational requirements often become immense. To solve this issue, high speed computation technologies such as quantum computing are becoming increasingly important.
There have been attempts to use quantum computers for structural analysis. One such attempt involves the use of quantum annealing, a method specialized in solving combinatorial optimization, for structural optimization of trusses [2]. However, quantum annealing is limited to handling binary variables of 0 or 1, which poses a problem when dealing with real numbers as it requires the combination of multiple qubits. This often exceeds the handling capacity of current quantum Ising machines, even for small analysis targets.
To overcome this limitation, our study adopts an alternative quantum computing approach, the quantum gate model. In a quantum gate model, the principle of superposition allows a qubit to take on a superposition of multiple states. This characteristic enables the handling of extensive information with a smaller number of qubits, presenting a significant advantage.
QAOA is a quantum gate model algorithm that can solve combinatorial optimization problems, similar to quantum annealing. This algorithm could be particularly useful for application in Noisy Intermediate-Scale Quantum (NISQ) devices. The state can be determined with fewer measurements by properly acting the shift operator [3]. In our research, QAOA is used to perform deformation analysis on truss structures, and the goal is to efficiently perform quantum computations and to demonstrate its effectiveness.

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Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ELASTOPLASTIC COMPUTING SAINT-VENANT FLEXURE-TORSION AND WARPING TORSION IN THREE DIMENSIONS

Hong-Ki Hong[*1] and Hsien-He Huang*[1]

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ABSTRACT

A prismatic rod of arbitray cross section shape --- singly or multi-connected solid sections, open or closed thin-walled sections, even multi-cell sections --- is studied. For this rod the Saint-Venant flexure-torsion theory is unified with the theory of warping moment and warping torsion, allowing the stress function and warping function to vary along the axial direction and establishing formulae between warping moment and axial stresses. A case study of H shape illustrates the variation of warping moment (i.e. the so-called bimoment), axial stresses, warping torsion, and warping displacements.

The centroid for axial force and the shear center for transverse forces are investigated both for thin-walled sections and for solid sections. The computation excuted for the rod made of elastic material is further extended to flow elastoplastic material modeled by an evolving cubic distortional yield hypersurface with a normality plastic flow and combined isotropic-kinematic rule of hardening-softening.

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Computational methods for wind energy
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPLORING THE USE OF METAMATERIALS TO MITIGATE VORTEX INDUCED VIBRATIONS OF WIND TURBINE BLADES

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[2]International Center for Numerical Methods in Engineering (CIMNE)

ABSTRACT

The historical upscaling of horizontal axis wind turbines has presented significant engineering challenges, including a heightened susceptibility to aeroelastic instabilities such as Vortex Induced Vibrations (VIV) [Horcas et al. (2022)]. This work explores, for the first time, the use of Locally Resonant Acoustic Metamaterials (LRAM) [Roca et al. (2019)] for the mitigation of such phenomenon on rotors. LRAM are composed of a regular array of lightweight repeating unit cells, each containing one or more resonators that can vibrate in response to external forces. The present work casts the targeted aeroelastic instability as a two-dimensional problem, consisting of a blade section connected to an elastic mounting. The flow is modeled using a computational fluid dynamics finite volume code. The structural properties of the mounting are obtained through modal analysis of a reference blade, and the effect of the local resonators is subsequently included. A partitioned fluid-structure interaction strategy is then employed to solve both physics in the time domain. The presentation analyzes the impact of the proposed metamaterial on the aeroelastic mechanism and sheds light on the potential of such an approach for vibration mitigation. However, additional work is anticipated to further assess the benefits of the technology, including the consideration of three-dimensional effects and the explicit modeling of the local resonators.

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Contact and interface mechanics: Modeling and computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MICRO-CONTACT MECHANICS WITH SOFT PARTICLE IN TRIBOLOGY

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ABSTRACT

This study focuses on establishing the establishment of the tribological analysis method for the machine parts when soft particles enter the machine part interface, their influence on tribological characteristics and their detection methods, and constructs a theoretical framework for soft particle interaction at the three-body contact interface, including its influence and detection methods. The detection technology can be used as a reference for future smart manufacturing. There are three main research results completed in this year: (1) Derived the three-body contact formula for soft particles, which establishes the relationship between external force, real contact area, and separation. This formula serves as a fundamental theoretical framework for interpreting experimental results and guiding future development of nano-lubricants. (2) Established a wedge-shaped relationship between real contact area (At/An) and load (F/AnE) at the three-body contact interface. The upper limit represents surface-to-surface contact, while the lower limit represents surface-to-particle contact. The height of this wedge is primarily influenced by surface roughness, with smaller roughness leading to a higher wedge value. (3) Employed a four-ball tribotester to analyze changes in tribological performance after introducing particles into the machine part interface. Results revealed a rapid increase in wear with increasing particle weight percentage. For an interface containing 1.48 wt% particles, the pitting area was 6.6 times larger compared to the particle-free interface. (4) Preliminary vibration measurements suggest a close and positive correlation between wear/pitting growth and MF4 values.

Boundary element methods: New theories and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TIME-DEPENDENT FUNDAMENTAL SOLUTION FOR NUMERICAL MODELING OF FOURIER AND NON-FOURIER BIOHEAT TRANSFER

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ABSTRACT

Numerical modeling of bioheat transfer has proven to be a powerful tool for predicting the thermal behavior of biological tissue in various medical fields. Currently, the Pennes model [1] is most commonly used for modeling bioheat, mainly because it is comparatively straightforward to implement and assumes an infinite speed of the heat wave. However, recent research shows that heat propagates at a finite speed in materials that have a cellular or inhomogeneous structure [2], resulting in a pronounced time lag between the temperature gradient and the heat flux. For this reason, non-Fourier models, such as the MCV model [3] based on the research of Maxwell, Cattaneo and Vernotte, have been developed.

In this presentation, a novel in-house algorithm based on the subdomain boundary element method for the numerical solving of bioheat transfer in biological tissue is presented, taking into account the Fourier and non-Fourier models of heat transfer, with the novelty being the implementation of the time-dependent (parabolic) formulation, which increases the accuracy of the solution compared to the elliptic formulation. The algorithm was verified using analytical examples and validated with experimental results from the literature. From the results, we can conclude that the developed algorithm successfully solves both Fourier and non-Fourier heat transfer problems.

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Recent advances in high-order methods for computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADAPTIVE SPACE-TIME MESH REFINEMENT FOR INCOMPRESSIBLE FLOWS

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ABSTRACT

This talk presents an adaptive mesh refinement technique for space-time finite element methods. The mesh adaptation can refine and coarsen the spatial mesh, therefore limiting the number of elements in a time-dependent simulation. Throughout the simulation, the spatial mesh, consisting of triangles, undergoes a red-green-blue refinement/coarsening step at every time level, and the space-time mesh, consisting of tetrahedra, is created by connecting the original and the updated meshes. The tetrahedral meshes guarantee that for incompressible flows, the solutions obtained by the space-time embedded/hybridized discontinuous Galerkin method are pointwise mass conserving and pressure robust. Numerical simulations will be presented to demonstrate the effectiveness and efficiency of the proposed method.

Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RESPONSE OF STREAMWISE VORTICES TO BLOWING AND SUCTION CONTROL IN TURBULENT CHANNEL FLOW

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ABSTRACT

Turbulent frictional drag constitutes a significant component of fluid drag in wall turbulence, and the opposition control [1] is a reasonable turbulence control strategy for reducing friction drag. This control method aims to counteract vortices near the wall that induct turbulent friction drag, through blowing and suction from the wall. Specifically, the velocity (v) in the wall-normal direction on a horizontal plane slightly away from the wall is detected, and an opposite velocity (-v) is imposed from the wall. However, the opposition control does not individually address numerous vortices in turbulence. The control also detects fluid motions other than streamwise vortices on the sensing plane, and the blowing and suction is applied to them. By forcusing on the dynamics of vortices, we anticipate even more efficient turbulence control.

The present study concentrates on the developing and decaying process of vortices. Vortices were identified by the second invariant II of the velocity gradient tensor, and their development/decay was assessed using the substantial derivative DII/Dt. Based on these values, streamwise vortices were statistically sampled in a direct numerical simulation of a fully developed turbulent channel flow over a sufficient time period. These sampled vortices were imposed with blowing and suction from the wall, inspired by the opposition control, and their responses were investigated.

The opposition control was applied on the sampled vortices, and their temporal evolution was tracked. The results revealed that the opposition control damped the vortices. However, there was no significant difference in the time required for the vortices to disappear entirely with or without control. Subsequently, the sampled vortices were subjected to either blowing ($v > 0$) or suction ($v < 0$) control. The findings indicated that blowing flow decayed the sampled vortices, whereas suction flow did not affect them. A control strategy based on these findings would be applied to the turbulent channel flow. We will discuss the details of the effect of blowing and suction on vortex dynamics and evaluate drag reduction rates.

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Imaging-based methods in computational medicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMAGE-GUIDED SUBJECT-SPECIFIC MODELING OF GLYMPHATIC TRANSPORT AND AMYLOID DEPOSITION.

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ABSTRACT

The glymphatic system is a brain-wide system of perivascular networks that facilitate exchange of cerebrospinal fluid (CSF) and interstitial fluid (ISF) to remove waste products from the brain. A greater understanding of the mechanisms for glymphatic transport may provide insight into how amyloid beta (Aβ) and tau agglomerates, key biomarkers for Alzheimer's disease and other neurodegenerative diseases, accumulate and drive disease progression. In this study, we develop an image-guided computational model to describe glymphatic transport and Aβ deposition throughout the brain. Aβ transport and deposition are modeled using an advection-diffusion equation coupled with an irreversible amyloid accumulation (damage) model. We use immersed isogeometric analysis, stabilized using the streamline upwind Petrov-Galerkin (SUPG) method, where the transport model is constructed using parameters inferred from brain imaging data resulting in a subject-specific model that accounts for anatomical geometry and heterogeneous material properties. Both short-term (30-min) and long-term (12-month) 3D simulations of soluble amyloid transport within a mouse brain model were constructed from diffusion weighted magnetic resonance imaging (DW-MRI) data. In addition to matching short-term patterns of tracer deposition, we found that transport parameters such as CSF flow velocity play a large role in amyloid plaque deposition. The computational tools developed in this work will facilitate investigation of various hypotheses related to glymphatic transport and fundamentally advance our understanding of its role in neurodegeneration, which is crucial for the development of preventive and therapeutic interventions.

Machine learning and data driven based engineering computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT OF A HYBRID MODEL FOR BATTERY ELECTRODE PRODUCTION WITH A PHYSICS-INSPIRED DATA-DRIVEN APPROACH

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ABSTRACT

Development of a Hybrid Model for battery electrode production with a physics-inspired data-driven approach
Somayeh Hosseinhashemi, Christoph Thon, and Carsten Schilde
Institute for Particle Technology (iPAT), Technische Universität Braunschweig

Process development in the industry is primarily based on trial and error and often involves expensive and time-consuming experiments. Typically, simulation analyses are used to build a process model. However, the simulations cannot always consider the manufacturing process's limitations in their modeling. Therefore, the process parameters determined by such a model remain almost theoretical. Alternatively, artificial intelligence methods can be beneficial. The expression of the relationship between physical quantities is widely used in many fields. However, these relationships are quite complex for many systems, making it difficult for conventional methods to determine the correct model. This work uses a hybrid modeling technique, incorporating physics-based knowledge and data-driven techniques. The goal of this approach is to combine the accuracy and physical insight provided by physics-based knowledge with the flexibility and scalability of data-driven models.

To achieve this goal, we combine a deep neural network with a genetic algorithm to determine the existing physical relationships between the data and then estimate the final model for the system. More precisely, we set out to determine the symbolic expression for an unknown function f using a genetic algorithm. To do this, we created a table of data consisting of rows in the form {x1, ..., xn, y}, where y = f (x1, ..., xn). We first attempted to simplify the data by analyzing it and identifying dimensionless parameters. Next, we utilized a neural network to search for any underlying physical properties within the data. Finally, we employed the genetic algorithm to generate various symbolic functions, selecting the most accurate one as the final expression. The resulting function was then applied as a white-box model to predict the behavior of our system.
This hybrid model allows for a more comprehensive and accurate prediction of the performance of the battery electrode and thus can be used to optimize the production process and improve the performance of the battery.

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Fluid-structure interaction: Methods and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ON THE NUMBER OF SUBPROBLEM ITERATIONS PER COUPLING STEP AND MONITORING CONVERGENCE IN PARTITIONED FLUID-STRUCTURE INTERACTION SIMULATIONS

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ABSTRACT

In literature, the costs of strong (implicit) coupling schemes for fluid-structure interaction are typically assessed by the number of coupling iterations required per time step, while ignoring the internal iterations within the nonlinear subproblems. We demonstrate that the internal iterations have a significant influence on the computational cost of the coupled simulation. Particular attention is paid to how limiting the number of iterations within each solver call can shorten the overall run time, as it avoids polishing the subproblem solution using unconverged coupling data. Specifically, it is demonstrated that performing subproblem iterations until the solver is fully converged in each call does minimize the number of coupling iterations but does not lead to minimal computational time. Instead, under the assumption of constant subproblem iteration cost, the optimum is found by minimizing a weighted sum of both coupling and subproblem iterations.

When analysing the optimal choice of the coupling steps and the internal iterations of the non-linear solvers, the question automatically arises as to when a time step can be considered converged. A variety of convergence criteria exists, but they all compare a quantity representative of the change in interface data between successive coupling iterations, e.g., the interface residual, to a prescribed tolerance. The choice of this tolerance value is often ad hoc and based on experience. Moreover, its relationship to the tolerances of the subproblems is unclear and often not considered, even though the accuracy of the coupled simulation is inherently linked to that of the solutions of the subproblems. We address this shortcoming by discussing a newly introduced criterion that does not require the choice of a coupling tolerance but bases the convergence of the time step on the number of subproblem iterations to reach convergence. This not only eliminates the inconvenient choice of a coupling tolerance but also allows one to better judge the accuracy with which the subproblems should be solved. The new criterion can be applied to black-box solvers under the condition that they provide information on whether they have converged and on how many subproblem iterations have been run. Although the focus of this work is on fluid-structure interaction simulations, the criterion applies to any type of coupling of black-box solvers under the given minor condition.

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Recent advances in computational fracture mechanics and failure analysis
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

OVER-DETERMINISTIC METHOD AND ITS APPLICATION IN FRACTURE MECHANICS

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ABSTRACT

The over-deterministic method (ODM) is dedicated to calculate a small set of unknown coefficients from a large system of equations, by making use of a large number of data points. A displacement over-deterministic method (DODM) developed by Ayatollahi et al. has been employed by for calculating the stress intensity factors (SIFs) as well as the coefficients of the higher-order terms in the Williams' series expansions for cracked bodies. The ODM provides a great idea to easily obtain fracture parameters, combine with finite element method (FEM).

In our work, a stress over-deterministic method (SODM) has been proposed for calculating the SIFs and T-stress at the crack tip for pure mode I, pure mode II and I-II mixed-mode cracks under static and dynamic loads. The effectiveness and computational accuracy of the SODM are verified using static and dynamic numerical examples. The effects of the number of terms in Williams' series expansion, the number and location of the nodes selected around the crack tip, and the mesh around the crack tip on SIFs and T-stress are discussed in detail. Results indicate that the SODM is simple and efficient in calculating the SIF and T-stress at the crack tip under static and dynamic loads.

Moreover, benefiting from the core idea of the ODM, a generalized over-deterministic method (GODM) is proposed to determine the Young's modulus and Poisson's ratio of materials through cracked specimens. A number of numerical examples of specimens with pure mode I, pure mode II and I-II mixed-mode cracks are carried out to verify the effectiveness and feasibility of GODM. The accuracy between the GODM and the traditional uniaxial tensile method for obtaining Young's modulus and Poisson's ratio of materials is verified by experiments using 2024-T3 aluminum alloy. The effects of the term number of Williams' series expansion, the number and location of selected nodes near the crack tip on results are discussed in detail. Results show that the GODM method can effectively and accurately determine the Young's modulus and Poisson's ratio of materials through the cracked specimens.

Advances in neural operators for scientific modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

UNCERTAINTY QUANTIFICATION FOR MULTIFIDELITY OPERATOR NETWORKS

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ABSTRACT

We will look at multifidelity Deep Operator Networks (DeepONets) as a way to improve the accuracy of DeepONet training when faced with a dataset with high uncertainty. Training DeepONets requires large amounts of data, and noisy data can decrease the accuracy of the training. One solution is to use multifidelity DeepONets, which use two different datasets simultaneously to train more accurately. We will show that using multifidelity DeepONets to add a small amount of high fidelity data, or using physics-informed training, can provide more robust answers than using the high fidelity data, physics, or low fidelity data alone, and can overcome noise in the low fidelity data when accompanied by high fidelity physics.

Quantifying epistemic uncertainties for computational predictions
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BACKCALCULATION FOR DESIGN UNDER GENERAL UNCERTAINTY: AN INTRODUCTION AND A TUTORIAL

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ABSTRACT

Uncertainty surrounds the design of engineered systems. Two main contributors to this uncertainty are the as-yet unfinished decision making the system's design and variation in the operational environment of the system. Engineering design has evolved from using deterministic rules and safety factors, which can often result in grossly overengineered systems, through designs based on worst-case scenarios, which treat catastrophic events as having high likelihood of occurrence, to robust and reliable design, which uses probability theory to minimize the risk of arriving at an unwanted outcome during the deployment of the system.

Despite providing a sound framework for the treatment of random variations, which constitute aleatory uncertainty, traditional probability theory has been repeatedly shown to be an inadequate tool for the characterization and management of epistemic uncertainty. This is just uncertainty from the lack of knowledge, which abounds in design, especially in its conceptual and preliminary (C&P) stages. Real-world uncertainty requires a more general class of uncertain numbers, such as the mathematical interval, characterizing epistemic uncertainty and the probability box characterizing mixed epistemic-aleatory uncertainty.

During C&P design engineers must come up with a robust and safe product, despite sometimes massive uncertainty. This task is most commonly formulated as an inverse problem, that is, candidate designs are evaluated against a set of criteria, which may also be uncertain, and the ones meeting the criteria are admitted for further evaluation. Most of the computational tools used in C&P design are fast, parametric models with open code, which is amenable to dissection and alterations. Engineers may find it tempting, therefore, to use deterministic arithmetic rules to invert the computations and project backward the uncertain numbers. Such projections, however, lead to systematic violation of design targets.

To ensure systems designed under general uncertainty respect the safety and performance limits, engineers can use backcalculation. In this talk we present the principles of backcalculation and controlled backcalculation for general uncertain numbers. We provide a demonstrative case study and draw attention to some outstanding problems as future directions of research.

Industrial applications of IGA
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

POINT CLOUD-BASED IMMERSOGEOMETRIC FLOW ANALYSIS

Ming-Chen Hsu[*1], Monu Jaiswal[1] and Ashton Corpuz[1]*

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ABSTRACT

In this talk, a new point cloud-based immersogeometric flow analysis framework will be presented. This framework is designed for simulating structures whose design models and analysis meshes are difficult to obtain. The proposed framework utilizes photogrammetry to reconstruct 3D point clouds of structures from 2D images captured by portable devices such as cell phones and drones. Additionally, it employs an immersogeometric approach that can directly carry out flow analysis on the reconstructed point clouds. New stabilization and regularization approaches that improve the solution quality will be discussed.

Microstructures of chemically complex materials and their impacts on material properties from multiscale simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INTEGRATING FIRST-PRINCIPLES CALCULATIONS AND EMPIRICAL STUDIES FOR EXPLORING MECHANICAL, ELECTRICAL, AND OPTICAL PROPERTIES OF HIGH-ENTROPY MATERIALS

Wen-Dung Hsu[*1], Kai sheng Huang[1], Chen-Yun Kuan[1] and Yuan-Chun Chang[1]*

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ABSTRACT

This study explores the dynamic realm of high-entropy materials, known for their diverse and nearly equiatomic composition. Departing from traditional materials with variable chemical makeup, the adjustment of components in high-entropy materials offers a wide spectrum of possibilities for tuning their physical and chemical properties, marking an innovative trajectory in material development. Our investigation specifically delves into the phase stability and mechanical properties of high-entropy alloys and high-entropy carbon nitrides. Additionally, we address the often-overlooked electrical and optical properties in existing literature on high-entropy alloys. In semiconductor applications, the interplay between metallic materials and their electrical and optical characteristics is pivotal. Embracing the high-entropy concept allows for the identification of superior metallic thin film materials, exemplified by reflective coatings typically utilizing aluminum or gold layers. While aluminum faces challenges with oxidation and gold proves expensive, high-entropy alloys emerge as promising alternatives, providing materials for reflective coatings that are both oxidation-resistant and cost-effective. Shifting focus to wear-resistant coatings, conventionally reliant on metal carbides or nitrides to enhance mold durability, we introduce high-entropy carbon nitrides as potential game-changers in this domain. Strategic use of different metals to govern bonding characteristics between metal-carbon or metal-nitrogen enables the fine-tuning of their mechanical properties. This adjustment facilitates the customization of coating characteristics to suit diverse applications, highlighting a compelling frontier for development in the wear-resistant coatings landscape. In summary, this study illuminates the multifaceted nature of high-entropy materials and their potential applications. By navigating beyond the constraints of traditional materials, we unlock avenues for tailoring properties in high-entropy alloys and carbon nitrides. This research contributes to the broader understanding of the intricate interplay between composition and properties, offering insights that may reshape material development strategies in fields ranging from semiconductors to wear-resistant coatings.

BATTERY DEGRADATION DIAGNOSTICS: CHALLENGES, METHODOLOGIES, AND TESTING CAMPAIGNS

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ABSTRACT

Battery degradation diagnostics is focused on continuously monitoring lithium-ion batteries' state of health (SOH), encompassing the estimation of capacity and degradation parameters throughout the service life. The insights derived from SOH estimation are crucial in guiding health-aware maintenance and control decisions. This presentation will start with an overview of battery degradation diagnostics, followed by a tutorial-like discussion of state-of-the-art methodologies, and conclude with a review of long-term testing initiatives led by a collaborative team from Iowa State University and the University of Connecticut. Special attention will be given to applying physics-informed machine learning to automate degradation diagnostics for in-line inspection and online battery management system (BMS) applications. The methodologies will be illustrated through practical demonstrations using a long-term aging dataset from implantable-grade lithium-ion batteries.

Computational mechanics for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CRYSTAL PLASTICITY MODELING OF RESIDUAL STRESS, DISLOCATION DYNAMICS AND CRACKING IN ADDITIVE MANUFACTURING

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ABSTRACT

In metal additive manufacturing (AM), complex thermal histories, large temperature gradients, and rapid cooling rates can lead to high residual stresses, distinct dislocation structures and even cracks. The generation and evolution phenomena during the AM process are not fully understood due to experimental challenges. In our study, we develop a multiscale modeling approach to investigate thermal and residual stress formation at the grain scale during the laser powder-bed fusion process. This approach integrates temperature profiles from thermal-fluid flow simulations and polycrystalline structures from phase-field grain growth simulations into a thermal-mechanical crystal plasticity finite element model. This framework allows for detailed observation of microscale thermal and residual stress evolution in AM materials. Based on this modeling framework, the deformation and temperature histories can be extracted to observe the dislocation dynamics in AM process. We then apply a continuous dislocation dynamics (CDD) model within a dislocation-based crystal plasticity framework to simulate the dislocation behavior under thermal stress in representative grains. Additionally, we extend our research to investigate the origins of strain localization phenomena in AM materials under loading at the grain scale, which is associated with the dislocation density and residual stresses induced by the AM process. This model can also be further coupled with phase-field fracture method to investigate the causes of crack formation during the AM process, reflecting the effect of thermal stresses during solidification and cooling. This modeling framework emerges as a powerful tool for the microscale mechanical analysis of AM materials and lays the groundwork for future multiscale process-structure-property investigations.

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Multiscale modeling, analysis and numerical methods of material defect and inhomogeneities
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ON EFFICIENT SOLVERS IN DENSITY FUNCTIONAL THEORY AND THEIR APPLICATIONS

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ABSTRACT

Density functional theory has been playing an important role in numerical simulations of nano materials etc. In this talk, towards the efficiency of the numerical simulations, several novel numerical methods such as multi-mesh method, multiple-precision method, as well as mesh adaptivity techniques will be introduced based on a finite element framework. More specifically, in the multi-mesh method, two different approximate spaces are designed for the wavefunction and the Hartree potential, respectively. Such a technique can reduce the requirements for both the memory and CPU time simultaneously. In the multiple-precision method, the calculation on the Hartree potential will be implemented in the single precision first to speedup the simulation, and the double precision calculation will be implemented in the last round SCF iteration to guarantee the accuracy. The mesh adaptivity is an effective approach for the acceleration, we will introduce the progress on the error estimation technique. Plenty of numerical results would show the effectiveness of proposed techniques. We finally will discuss the potential application of our solver in the material simulations.

STRUCTURE-PRESERVING DISCRETIZATION OF INCOMPRESSIBLE MHD SYSTEMS AND IDEAL MAGNETIC RELAXATION

Kaibo Hu[*1]

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ABSTRACT

The magnetohydrodynamics (MHD) systems have several important conservative properties, e.g., the magnetic Gauss law and the conservation of energy and (magnetic, cross, hybrid) helicity in the ideal limit. These conserved quantities encode various kinds of intrinsic symmetry of the equations. To achieve physical fidelity and numerical stability, it is desirable to preserve these conditions precisely in the numerical discretization (up to the machine precision). In this talk, we first review the conservative properties of continuous MHD systems and the idea of Finite Element Exterior Calculus. Then we construct finite element methods that precisely preserve these properties. Discrete de Rham sequences play a vital role in the study. We also apply the idea to ideal magnetic relaxation.

Multi-scale and machine learning-based modeling methods for optimization and design of composites
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DYNAMIC AND STABILITY ANALYSIS OF PRESTRESSED THIN-WALLED FILAMENT WOUND GLASS FIBRE COMPOSITE CYLINDERS WITH METAL LINER

Ruiqi Hu[1], Ziwei Yuan[1] and Chao Zhang[1]*

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ABSTRACT

The cylindrical filament wound composite overwrapped shells with a metal liner have been widely used in spaceflight and nuclear fuel centrifuge rotors due to their high strength and low weight. However, optimizing the structure of these high-speed rotating cylinders is more complicated due to the counterbalanced factors of load-bearing capacity, structural stiffness, and servility stability, coupled with dimensional parameters and the filament winding process. To reveal the mechanism of the initial reinforcement effects of filament winding of GFRP on metal liner, including load sharing ability, stiffness and buckling capacity, this study proposes a filament wound GFRP, which offers a high strength-to-weight ratio compared to existing metallic material. The 3D finite element model is built using ABAQUS software to predict the dynamic and stability characteristics of circular cylindrical shells with fixed boundary conditions. The computation models are validated by comparing with reported results in previous literatures. The hybrid GFRP cylindrical shells is further studied by varying filament winding process parameters such as winding angle and stacking sequence. The reinforcement effect on the metal liner resulting from the filament wound was achieved by using the equivalent temperature drop method and the element birth and death technology. The critical circumferential stress in composite shell which protects the metal liner from plastic material failures and keep the minimum tension load inside the GFRP composite material during high-speed rotation condition is determined. The discrete assumption is employed to depict the critical buckling strength considering the external hydrostatic pressure force and the winding process effect, to shed light on the underlying mechanism principles behind the buckling strength of such hybrid structures. Moreover, to reveal the impact of design-related parameters on the structure’s natural frequencies and linear buckling strength, sensitivity analyses are conducted on structural thickness, rotation speed and pretensions in composite materials. It was found that although the critical buckling strength of the hybrid structure under hydrostatic pressure force is lower than the pretension-induced compression force, the structure is still free from buckling failure. In conclusion, determining the relative contributions from mass and stiffness facilitates the optimization of structural geometric parameters. The numerical analysis method can provide valuable suggestions for engineering applications and promote lightweight design and safety conditions.

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Transport phenomena in micro/nanofluids
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STRUCTURE-PERSEVERING METHOD FOR MECHANOELECTRICAL FLEXIBLE HUB-BEAM MODEL OF IONIC-TYPE SOLVENT-FREE NANOFLUIDS

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ABSTRACT

The liquid-like properties of ionic-type solvent-free nanofluids at room temperature can realize various advanced functions[1, 2], which has important applications. At present, the problems related to determining the critical flow conditions of solvent-free nanofluids are still unresolved. In this paper, the microscopic flow mechanism of solvent-free nanofluids is revealed from the perspective of kinetics. The vibration of the canopy and coronal layers of ionic solvent-free nanofluids can be excited by the external environment, which drives the rotation of the nanocore and shows liquid-like properties. Focusing on the microscopic mechanism, a mechanoelectrical flexible hub-beam model in a circular electric field is established for ionic-type solvent-free nanofluids. A structure-preserving method[3] combining generalized multi-symplectic and symplectic precise integration is constructed to simulate the dynamic behavior of ionic solvent-free nanofluids. The merits of the numerical method include the high precise and the structure-preserving characteristic, which implies that, the tiny rotation velocity can be captured and the liquid-like behaviors of ionic-type solvent-free nanofluids can be reproduced by the complex structure-preserving method exactly. The critical initial perturbation intensity of ionic solvent-free nanofluid flow is obtained from the numerical results, and the upper limit of flow velocity is confirmed, which provides an important guidance for the preparation and dynamic control of ionic solvent-free nanofluid.

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Mesh-free particle methods for multi-physics problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN SPH FORMULATION FOR GENERAL PLATE AND SHELL STRUCTURES WITH FINITE DEFORMATION AND LARGE ROTATION

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ABSTRACT

In this work, we propose a reduced-dimensional smoothed particle hydrodynamics (SPH) formulation for quasi-static and dynamic analyses of plate and shell structures undergoing finite deformation and large rotation. By exploiting Uflyand–Mindlin plate theory, the present surface-particle formulation is able to resolve the thin structures by using only one layer of particles at the mid-surface. To resolve the geometric non-linearity and capture finite deformation and large rotation, two reduced-dimensional linear-reproducing correction matrices are introduced, and weighted non-singularity conversions between the rotation angle and pseudo normal are formulated. A new non-isotropic Kelvin-Voigt damping is proposed especially for the both thin and moderately thick plate and shell structures to increase the numerical stability. In addition, a shear-scaled momentum-conserving hourglass control algorithm with an adaptive limiter is introduced to suppress the mismatches between the particle position and pseudo normal and those estimated with the deformation gradient. A comprehensive set of test problems, for which the analytical or numerical results from literature or those of the volume-particle SPH model are available for quantitative and qualitative comparison, are examined to demonstrate the accuracy and stability of the present method.

The phase field method for fracture: Theory, numerics, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ON REALIZING SPECIFIC FAILURE CRITERIA IN PHASE FIELD MODELS

Xiaofei Hu[*1], Weian Yao[1] and Zhi Sun[1]*

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ABSTRACT

Phase field model (PFM) can be viewed as an extension of classic energy competition the-orem proposed by Griffith, and can realize crack initiation and propagation without any ad-hoc criterion, which was considered as a merit of the phase field model. However, it may become an obstacle when a specific failure criterion is required in a specific problem calculation. In order to solve this issue, we propose a simple way to embed different failure criteria into the PFM in this work. On one hand, an activation parameter is introduced into the PFM's driving force to control the fracture timing. On the other hand, a structural tensor is introduced into the PFM's surface density function to reflect the fracture direction predicted by the specified criterion. The fracture evolution direction is enforced in line with the criterion through a penalty parameter. Several numerical examples are provided to testify our proposed method, and the comparison of our model with both the results from extended finite element method (XFEM) and experiments testify the effectiveness of the proposed model.

Multiscale, multifield, and continuum-discontinuum analysis in geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A 3D NONLOCAL HYBRID ELASTO-PLASTIC FRACTURE MODEL OF ROCK-LIKE MATERIALS

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ABSTRACT

In order to simultaneously describe the elasto-plastic and damage behaviors of rock-like materials under various pressure conditions, a 3D nonlocal hybrid elasto-plastic model based on three-dimensional Hoek-Brown criteria is proposed in this paper. The proposed model couples the non-ordinary state-based peridynamics (NOSBPD) method and the nonlocal differential operator method to eliminate the surface effect due to the incomplete integral region near the boundary, and to simplify the imposition of boundary conditions. A plastic constitutive model with the well-known three-dimensional Hoek-Brown criterion is integrated within this framework to accurately represent the nonlinear behavior of rock-like materials. Note, that the effect of intermediate principal stress on elastic-plastic fracture behavior is considered in this model. The segmented flow rule is used for different pressure conditions. Strain-softening and fracture criteria, based on the equivalent plastic strain, capture the elasto-plastic response and damage-fracture processes in rock. The dynamic relaxation method is combined with the return mapping method to address quasi-static nonlinear problems. The proposed model is verified by comparing its results with those from the Finite Element Method (FEM), as well as with experimental data from the literature. Numerical examples contain the triaxial compression tests and compression tests of rock specimens with pre-existing flaws. Numerical examples demonstrate that the proposed model captures well the entire elasto-plastic fracture process for rock-like materials, including elasto-plastic deformations, crack propagation and progressive failure.

Mathematical modeling and simulation for social, environmental, and disaster prevention issues
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPARISON OF VORTEX STRUCTURES AND TURBULENT HEAT TRANSPORT FOR A SINGLE JET AND MULTIPLE JETS IN CROSSFLOW FOR PREDICTION OF HOT AIR RECIRCULATION

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ABSTRACT

The flow pattern of the hot air discharged from Air-Cooled Heat Exchanger (ACHE) fans under the crosswind condition is similar to a single jet in cross flow (SJICF) or multi-jets in crossflow (MJICF). The understanding of the physics in SJICF and MJICF will help predict Hot Air Recirculation (HAR) phenomena for achieving more production increase of LNG plant. Large Eddy Simulation (LES) has been carried out for a single jet and five spanwise jets with the jet-to-jet spacing of 1.6 jet nozzle diameter. The jet to crossflow velocity ratio VR is 3.3 and the Reynolds number Re_c is 2100, based on the crossflow velocity and jet nozzle diameter. The numerical schemes used in this study can provide good prediction accuracy in mean velocity/temperature, RMS velocity fluctuation, and Reynolds stress.

A significant difference in the vortical structures, shedding frequency, and jet trajectory is found between the sing jet and multi-jets. Firstly, the counter-rotating vortex pair (CVP) is only formed in a very short distance and cannot evolve in the streamwise direction. The hanging vortex is found to be split into two disconnected parts. No coherent large-scale vortical structure such as wake vortex and horseshoe vortex legs can be observed behind the multi-jets except for a lot of small-scale wakes. The Proper Orthogonal Decomposition (POD) analysis reveals that the dominant shedding frequency of the shear layer vortex in the multi-jets increases to 32 Hz compared with 18 Hz in the single jet. Secondly, the comparison shows that the multi-jets penetrate 20% less into the cross flow. Thirdly, the interaction mechanism between adjacent jets is revealed in this study. The analysis of sampling data in the flow path between the jets shows that the flow in the jet-to-jet spacing behaves as a pulsating jet flow with a frequency of 32 Hz. The width of the flow path in the spanwise direction shrinks and expands alternately causing the fluctuation in the streamwise velocity, which subsequently generates a lot of small wakes to the jet downstream.

The feature of the turbulent heat transport in multi-jets is revealed. It is found that the time-averaged turbulent heat flux in the vertical direction is larger in the jet-to-jet border because of the interaction while the time-averaged turbulent heat flux in the streamwise direction is larger at the jet rear because of the velocity acceleration in the multi-jets body.

ON NONLOCAL CONTINUUM MECHANICS OF FINITE STRAIN BOND-BASED PERIDYNAMICS

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ABSTRACT

Peridynamics (PD) is a non-local continuum mechanics theory over two scales, where the macro-scale material responses are built based on the interaction forces among meso-scale material points. Unlike molecular dynamics, where the pairwise bond forces consist only of normal components along the bonds, our recent research demonstrated that the pair-bond force of peridynamics can include both normal and tangential components to capture macroscale material responses without introducing micro-polar continuum theory. In this study, we systematically developed a consistent finite strain nonlocal continuum theory based on a consistent and compatible bond-based peridynamics formulation that incorporates interactions in both normal and tangential directions among material points. A key feature of the proposed formulation is the alignment of meso-scale bond deformation with the finite-strain deformation theory, resulting in a meso-scale pairwise bond potential that is compatible with the finite strain energy density of macro-scale cohesive continuum. In contrast to conventional bond-based peridynamics and recently proposed extended-bond-based peridynamics which calculate relative displacements of bonds in a manner akin to structural truss elements, the proposed formulation uses the finite deformation strain measure, specifically the Green-Lagrange strain, as its primary deformation measure. This allows the finite strain bond-based peridynamics to capture the full spectrum of material deformation, including tension, shear and torsion, making it suitable for both infinitesimal and finite deformations in nonlocal continuum mechanics. Notably, our proposed formulation completely resolve the issue of zero-energy modes that inherently and persistently existence in the current peridynamics formulations. Moreover, utilizing the proposed formulation enables us to derive the general non-local stress measures through a standard mathematical procedure. The proposed novel peridynamics formulation cohesively integrates all essential elements of non-local continuum mechanics, kinematics, constitutive relation, governing equations, into one unified framework. Numerical examples, covering a range of problems from elasticity to nonlinear fracture, are provided to demonstrate the effectiveness of the proposed formulation.

New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A STABILIZED FRAMEWORK FOR NONLINEAR TOPOLOGY OPTIMIZATION BASED ON TIME-SERIES MOVING MORPHABLE COMPONENTS METHOD

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ABSTRACT

The topology optimization of structures under large deformation has long been a challenging problem lacking stability during iteration. Getting the responses of every possible topology is the biggest challenge for this problem. For the density-based topology optimization, a linear interpolation scheme for the voids is introduced to enhance the stability of iteration. However, instability caused by the gray elements still persists. The explicit feature of the moving morphable components (MMC) method endows a good control of gray elements in the design space and hence has potential advantages in the problem under large deformation. This paper introduces the time-series moving morphable components method to solve the nonlinearity topology optimization problems. To further enhance the stability during iteration, various strategies are proposed. A direct modification of nonlinear strain is proposed to adress the instability caused by voids. The buckling control strategy is introduced to eliminate the instability caused by slender components. Further, the global-local mixed design variable as well as the trust-region based moving asymptotes optimizer are adopted to eliminate the instability of iteration reported in the traditional MMC framework.

Advanced analysis of steel and steel-concrete composite structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INVESTIGATION OF STRESS IN LINK SLABS OF JOINTLESS STEEL-CONCRETE COMPOSITE BRIDGES

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ABSTRACT

Jointless steel-concrete composite bridges have been widely applyed due to their merits of fully utilizing the mechanical properties of both steel and concrete and of getting rid of expansion joints by link slabs. Well link slab detailing, therefore, is crucial for their successful application. This study focuses on the analysis of transverse stresses in the link slab of a jointless steel-concrete composite bridge. By employing linear elastic theory of plate, the deflection and stress distribution functions of the link slab are determined. The validity of the close solution was first verified with both numerical simulation and load testing. The results indicate that the upper face of the link slab, located at the end of the steel girder, experiences the highest tensile stress in both transversal and longitudinal directions of the bridge. Furthermore, the impact of the link slab's area size on the peak stress in the transversal direction of the bridge is investigated. It is indicated that smaller spacing and longer end length of longitudinal beams lead to an increase in the maximum transversely tensile stress in the link slabs, resulting in the initiation of cracks before reaching their design loads. Therefore, for jointless steel-concrete composite bridges, transversal stresses must be considered in the link slabs except for longitudinal stress investigation.

Data-driven device and circuits models
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT AND TESTING OF SUBCIRCUIT SURROGATE MODELS USING DATA-DRIVEN EXTERIOR CALCULUS AND XYCE-PYMI

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ABSTRACT

We evaluate data-driven surrogate models of subcircuits within the model-based design paradigm. Our goal is to design subsystem models that offer fidelity when integrated in a larger system, ensuring that systems designed using the surrogate models perform as expected when built. Physics-based constraints that augment data-driven methods are advantageous for intelligent, validated, and credible model-based design. The Data-Driven Exterior Calculus can be applied to learn subcircuit surrogate models based on deep neural networks that obey physical constraints such as Kirchoff's current law. These Python-based subcircuit models can be trained using imported from Xyce simulations, then reintegrated into the Xyce workflow as devices within Xyce-PyMi. We demonstrate training and evaluation results within this workflow on several direct current examples that are of broad interest as benchmarks and based on national lab circuit designs. We discuss best practices for training the surrogate models, which may be sensitive to architectural choices and hyperparameter values.

Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HEAT TRANSFER ANALYSIS OF VORTEX-RING COLLISIONS WITH A VERTICAL CONSTANT-TEMPERATURE WALL BASED ON DNS

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ABSTRACT

The impact of vortex rings generated by impinging jets plays a significant role in heat transfer processes. However, the simulation of such phenomena poses Challenges in mesh resolution and computational accuracy due to the involvement of complex multi-scale flow effects. This study introduces a high-resolution direct numerical simulation (DNS) approach, employing the Fast Fourier Transform (FFT) and the Semi-Implicit Method for Pressure Linked Equations (SIMPLE), to investigate the interaction between vortex rings and a vertical wall. The research is based on the DNS results to explore the coupling effects between the boundary layer and vortex rings, along with secondary vortices. It includes an examination of secondary vortex formation and evolution in different spatial regions, as well as the flow structure under varying Reynolds numbers. The study provides a comprehensive analysis of the flow dynamics, exploring the intricate patterns and interactions that occur during the collision of vortex rings with the wall surface. Moreover, the investigation delves into the effects of different flow states on boundary heat transfer. Numerical results illustrate that the high-resolution DNS, combining FFT and SIMPLE, has effective in capturing the detailed physics of vortex-wall interactions.

Mesh-free particle methods for multi-physics problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A COUPLED SPH-FDM METHOD FOR SIMULATIONS OF UNSTEADY FLOWS

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ABSTRACT

Smooth particle hydrodynamics (SPH) has significant advantages in the flows with the moving boundary or the free surface, however it is often limited due to its expensive computational cost. Finite particle method (FDM) is convenient to implement multi-resolutions, so it is usually high efficient. A coupled SPH - FDM is proposed to simulate the unsteady flows with the moving boundary or the free surface. The coupled SPH - FDM can solve fluid equations in Euler coordinate system [1] or Lagrangian coordinate system [2]. For Euler coordinate system, the overlapping particles and grid nodes are created near the interface between particles and grids in order to exchange the information of two methods, and the shifting particle technology is applied into simulations to adjust the positions of the particles for matching the movement of the boundary. For Lagrangian coordinate system, as well as the overlapping particles and grid nodes and the shifting particle technology, the creation (or deletion) of particles is introduced into the simulations to maintain the numerical stability. Euler coordinate system is usually convenient to simulate the flows around the moving body in a closed computational domain while Lagrangian coordinate system is convenient to simulate the flows with the free surface or the multi-phase flows. Some classical unsteady flows or applications are simulated and the results are compared with literature or experimental results to verify the accuracy of the coupled SPH-FDM.

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Data science and machine learning applications for composite materials and biomedical engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INVESTIGATION THE OF GRAIN SIZE EFFECT OF NANOGLASS USING A MESOSCALE MODEL WITH VARIABLE CHARACTERISTIC STRAIN

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ABSTRACT

Nanoglass, composed of heterogeneous glassy domains created by introducing interfaces into metallic glasses at the nanoscale, could be a promising strategy against severe shear localization, as demonstrated by a series of atomistic simulations. In this study, a mesoscale morphological model based on the kinetic Monte Carlo (kMC) algorithm is used to investigate the effect of grain size on nanoglasses (NGs). Considering that the development of shear bands during deformation can be categorized into four stages according to the aged-rejuvenation-glue-liquid model, we propose a variable characteristic strain (VCS) based on a sigmoid function to capture this process. Our simulations reveal that a transition from inhomogeneous to homogeneous deformation occurs as the NG grain size decreases to approximately 10 nm. This transition is attributed to the impediment of shear band formation by the small grain size, leading to strain hardening. The critical grain size predicted by our mesoscale model is in good agreement with molecular dynamics simulations. Furthermore, a progressive reduction of elastic constants is introduced to characterize the failure response. Numerical examples demonstrate that our kMC model is valuable for designing NGs to counteract shear localization, particularly when the appropriate VCS can be obtained from atomistic simulations.

16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Advancements in model reduction, data assimilation, and uncertainty quantification for complex physical systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FEATURE-DRIVEN SAMPLING STRATEGY IN ADAPTIVE MODEL ORDER REDUCTION FOR SHOCK-DOMINATED PROBLEMS

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ABSTRACT

Physical problems featuring strong shock advection (e.g., hypersonic flows and detonations) often present significant challenges and are well-recognized to be not amendable for conventional model-order reduction (MOR) methods. This can be mainly attributed to the well-known issues associated with the slow decay of Kolmogorov N-width. In literature, several remedies have been proposed to address this challenge via local subspaces, nonlinear manifolds, or adaptive MOR. In the current work, we focus on establishing an adaptive MOR methodology to construct reduced-order models (ROMs) for shock-dominated problems. In general, the adaptive MOR techniques seek to update the subspace in the online stage to satisfy an optimal representation of the evaluated dynamics in the target problems. One of the most crucial factors in adaptive MOR is the sampling points/locations selection for dynamics evaluations to minimize the posterior errors in representing the target physics. Therefore, specifically in this work, we develop a feature-driven sampling strategy to identify and select points near the shock wave fronts in adaptive MOR to improve the predictive capabilities of the resulting ROMs. Two canonical shock problems are considered to assess the proposed sampling strategy: 1) a sod shock tube; and 2) a 1D detonation tube.

SciML in the real world
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FP-IRL: FOKKER-PLANCK-BASED INVERSE REINFORCEMENT LEARNING - A PHYSICS-CONSTRAINED APPROACH TO MARKOV DECISION PROCESSES

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ABSTRACT

Seemingly identical cells in a biological system exhibit distinct responses to the same environmental cues, so how are heterogeneous behaviors being provoked? There is a lack of a systematical method to understand the behavior of a single living agent (e.g. cells) in a complex biological system. The current modeling approach utilizes partial differential equations that build upon the Markov process without considering the possibility of the decision-making process in a living agent and the quantitative causality between decisions and states. In contrast, we employ Markov decision processes to characterize living agents in biological systems as intelligent agents that can make decisions following a policy that maximizes the expected cumulative reward. The reward function encapsulates the incentive mechanism and quantifies the motivation of the agent’s behavior. This will establish a new paradigm for studying complex behaviors in multiple biomedical systems. The reward structure driving the decision-making of an agent is generally unknown. To help uncover the motivation behind the behavior of the living agent, we leverage Inverse Reinforcement Learning (IRL) to estimate this unknown reward function from observation data of the studied agent. Like other inverse problems, IRL is typically ill-posed and becomes especially challenging when the transition model is unknown or inaccessible for sampling because the evolution of states and actions depends both on the transition model and the agent's policy, which is derived from the transition model as well together with the reward function. Conventional IRL approaches either assume the transition model is accessible or utilize data-driven methods to estimate the transition model beforehand without considering physics. We propose a novel physics-aware IRL algorithm that can simultaneously infer the reward function and transition probability function from observed temporal data. We first establish a connection between the reward function in IRL and the potential function in the Fokker-Planck equation (FPE), a partial differential equation that governs the time evolution of the probability density of the agent's states. Next, we employ variational system identification to infer the potential function in FPE, which in turn allows the reward, policy, and transition probability functions to be evaluated instantaneously leveraging the established connection. In addition to obtaining the reward function, new cell states and decisions can also be predicted and simulated as the state transition is mathematically modeled. We demonstrate our approach using a Gridworld benchmark problem and a cancer cell migration problem.

Advances in damage & fracture modeling of multiphysics materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A FULLY COUPLED THERMO-MECHANICAL LOCALIZING GRADIENT DAMAGE MODEL WITH A MODIFIED MAZARS STRAIN

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ABSTRACT

Thermal crack is a common thermomechanical coupling phenomenon in both natural and engineering situations, such as the drying of soils, the shrinkage of concrete, and the quenching test of ceramics. The bidirectional thermo-mechanical coupling exerts a substantial influence on crack patterns, especially in situations sensitive to temperature variations. Besides, varying constraints give rise to tension or compression zones within the material, leading to distinct modes of thermal cracks. Comprehensively describing the thermomechanical coupling effects and accurately capturing different failure modes remain challenges in thermal crack modeling. To address this issue, a thermodynamically consistent and fully coupled gradient damage model is proposed based on a differential form of non-local damage theory. This model is designed for thermal cracks in both quasi-static and dynamic scenarios, and it accurately characterizes the impact of thermal expansion on the stress field and the contribution of volumetric strain and damage evolution to the temperature field. Furthermore, to precisely describe different modes of thermally induced cracks, a modified Mazars strain is formulated as the driving force for the gradient damage model, which introduces the first invariant of the strain tensor and the tension-compression strength ratio to the traditional Mazars strain. The numerical results confirm the reliability of the modified Mazars strain in capturing different modes of failure and demonstrate the capability of the proposed damage model to characterize complex damage patterns under thermal loading in both quasi-static and dynamic scenarios. Additionally, in the simulation of the quenching test of ceramic plates, traditional models, which ignore the influence of volumetric strain and damage evolution on the temperature field, tend to overestimate temperature changes, resulting in fewer cracks and larger crack spacing compared to experimental results. While the proposed fully coupled damage model aligns well with experimental results. In the simulation of thermal shock on cylindrical specimens, the damage pattern is found associated with compression strength, which transfers from spiral shear bands to a halo-like annular damage zone and radially developed damage.

PARAMETER IDENTIFICATION OF PIEZOELECTRIC ENERGY HARVESTER BASED ON ISOGEOMETRIC ANALYSIS VIA BAYESIAN UPDATING

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ABSTRACT

The piezoelectric energy harvesters (PEHs) have been widely studied in recent years, with various models employed to simulate their dynamic behavior. However, the accuracy of these models is often affected by uncertainties arising from both manufacturing and operational factors [1]. This work aims to identify the most probable input parameters of the model based on nominal value to align numerical results with experimental results, considering the above-mentioned uncertainties. In this work, a Kirchhoff-Love plate model utilizing isogeometric analysis (IGA) [2] is employed to generate numerical Frequency Response Functions (FRFs) of PEHs, which are then compared with experimental FRFs. The Bayesian updating is the key technique applied to find out the most likelihood parameters by the posterior probability function which is obtained from the Transitional Markov Chain Monte Carlo (TMCMC) algorithm. Additionally, given the increased number of input parameters associated with the plate model, a model class selection study is also conducted to find out the most appropriate group of parameters for Bayesian updating. The study tests a total of 5 devices with different widths, 4 of which are cut from a standard commercial PEH. The results from the model class selection show that parameters of piezoelectric material and geometry properties will have higher uncertainty. This uncertainty is primarily due to the thin structure of PEHs, leading to variations of PEH properties during manufacturing and the cutting process to obtain different sizes of PEHs. Furthermore, Bayesian model updating effectively identifies key parameters, matching numerical FRFs with experimental results. Updated parameters also perform well in an extended Multi-PEHs model, showing good agreement with experimental data from coupled devices. In the future, a direct model updating on the Multi-PEHs model will proceed for further comparative analysis.

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Imaging-based methods in computational medicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INCORPORATING ANISOTROPIC MATERIAL MODELS INTO AUTOMATED IMAGE-BASED MODELING AND MESH GENERATION FOR VASCULAR FLUID-STRUCTURE INTERACTION

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ABSTRACT

This study presents a refined framework for vascular modeling and mesh generation to enhance the accuracy of vascular Fluid-Structure Interaction (FSI) simulations. The method begins with the acquisition and preprocessing of medical images to construct a three-dimensional representation of vascular structures. This underpins the ensuing arterial wall constitutive model[2].

A crucial aspect of our methodology is the computation of the vascular centerline, imperative for delineating complex vascular network geometries and ensuring accurate 2D segmentation of blood vessels. We utilize a deep learning algorithm to extract 3D vascular lumen segmentation from medical images, followed by an efficient method[1] for centerline and radius computation. This approach is convenient and cost-effective compared to traditional methods without loosing accuracy in capturing the vascular network.

Our methodology advances vascular wall model generation and mesh generation through the application of scaling and lofting techniques based on the lumen geometry. It circumvents the limitations of traditional extrusion-based methods.

A fundamental aspect of our approach is the establishment of a local basis within the vascular tissue, due to the anisotropic properties of biological tissues[2]. We define a local basis at each mesh node, which is informed by the vessel's morphology and the derived centerline data. This technique is particularly appealing for patient-specific vascular structures. Through simulations of idealized curved geometries and two-layered abdominal aorta models, our method proves to be more robust and accurate than the existing elasticity-based method, especially in regions with varying diameters and bifurcations, highlighting the importance of anisotropic arterial wall models in vascular FSI.

Our approach, integrating advanced image processing, precise segmentation, and sophisticated mesh generation, performs well in defining fibers in patient-specific models. This technology suite advances vascular modeling and thus enhance the pipeline of image-based simulation.

Keywords: Segmentation, Centerline, Vascular modeling

Reference

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Data-driven approaches for solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STUDY ON GAS ADSORPTION BEHAVIOR IN SHALE NANOPORES BASED ON MOLECULAR KINETIC THEORY AND MACHINE LEARNING METHOD

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ABSTRACT

Understanding the shale gas adsorption behavior in shale nanopores is essential for the reservoir estimation of shale gas, and understanding the competitive adsorption behavior of CO2 and CH4 in shale nanopores is crucial for enhancing the recovery of shale gas and sequestration of CO2. Considering the complexity of geological environment and nanoporous structure of shale, traditional methods based on experiments and molecular dynamics simulations are always expensive and inefficient. In our work, we analyzed and predicted the adsorption behavior of shale gas and the competitive adsorption behavior of CO2 and CH4 by combining microscopic analysis methods and machine learning methods, respectively. One the one hand, a machine learning framework to predict the methane adsorption behavior in shale nanopores is constructed from the microscopic and kinetic theory perspectives, where some novel parameters related to potential energy distribution are proposed to represent the methane adsorption characteristics of shale slit nanopores. Machine learning model based on the uniformly constructed dataset is introduced to realize fast and accurate prediction of methane adsorption behavior, which is well validated by typical inorganic and organic models. On the other hand, the theoretical connection between inherent characteristics of molecules and adsorption behavior is built to reveal the general laws in the behavior of CO2/CH4 competitive adsorption through posture analysis of the molecules. A machine learning algorithm, aided by molecular kinetic theory, is proposed to facilitate the fast and accurate predictions of competitive adsorption behavior, and detailed analyses of the influencing factors are conducted accordingly. The insights gained from our work provide a foundation for expeditiously estimating the competitive adsorption behavior of CO2/CH4, with potential implications for CO2 sequestration and enhanced gas recovery process, and would be beneficial for the exploitation and development of shale gas reservoirs.

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Battery modeling and computation: From material to device
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPERIMENTAL CHARACTERIZATION AND NUMERICAL MODELING OF DEFECTIVE BATTERY CELLS INDUCED BY MECHANCIAL ABUSE

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ABSTRACT

In challenging operational environments, lithium-ion batteries (LIBs), as cutting-edge power sources for diverse applications, inevitably endure external loads like impact and extrusion, posing risks of battery damage and failure. Consequently, investigating the safety performance of LIBs under mechanical loading becomes a central focus in LIBs research. Simultaneously, the concept of cascaded utilization is introduced to maximize the remaining value of retired batteries and alleviate recycling pressure from discarded batteries. Hence, before recycling and reusing batteries, especially older models or damaged ones, a thorough assessment of their electrochemical performance, safety risks, and the implementation of targeted design controls and management algorithms are crucial. This is integral to achieving efficient energy storage device utilization and ensuring overall safety throughout the battery lifecycle. To achieve a more accurate electrochemical analysis and prediction of damaged batteries, this study conducts relevant experimental characterization and numerical modeling. In the experimental section, the impact of low-velocity impacts on the performance and safety of LIBs, influenced by electrochemical cycling and dynamic loading, is explored. Various conditions, such as impact energy, State of Charge (SOC), and C-rates, systematically reveal mechanical, electrochemical, and thermal responses, as well as damage behaviors. The study demonstrates that higher impact energy leads to increased structural stiffness, maximum temperature, and maximum voltage drop. Additionally, heightened impact energy and SOC significantly influence electrochemical parameters, including charging capacity and internal resistance. In the simulation section, for a more precise mechanism explanation and parameter analysis through numerical simulations, it is essential to consider the distribution of current and Li concentration, including the inherent structural non-uniformity of the cell, as well as geometric and material non-uniformities. The uneven charge distribution resulting from these non-uniformities has been identified in previous studies as a significant factor contributing to battery cycling performance degradation and a reduction in safety. In this work, the focus is on electrode-level non-uniformities introduced by battery structure and electrode accidental deformation damage. We investigate the impact mechanisms of intra-electrode non-uniformities on the electrochemical performance and safety of batterie aiming to elucidate the quantitative relationship between non-uniformities and the extent of performance degradation. The methodology and experimental findings provide insights for enhancing safety design, conducting risk assessments, and enabling the cascading utilization of energy storage systems based on LIBs.

Keywords: Lithium-ion battery; Low-velocity impact; Damaged battery; Cycling performance; Battery modeling

Design and mechanics of mutifunctional composites and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STRUCTURAL DESIGN AND EXPERIMENTAL ANALYSIS OF PORTABLE ROPE-CLIMBING ROBOT

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ABSTRACT

For the extreme environments such as special combat, high altitude operation, earthquake rescue and other extreme environments, the manual operation is difficult, high operating cost, high risk factor, and the traditional rope climbing robot fixed the power system and transmission system in advance at the end point of the operation, the operation area is fixed and inefficient. Therefore, based on the optimized design of rope-sheave lifting mechanism, a portable rope-climbing robot is designed. The flexible rope is used as the transmission medium, which is wrapped around the inside of the rope-climbing robot, one end of which is fixed at the end of the transmission, and the other end of which is freely suspended, and the friction between the rope and the rope-sheave is used as the motive force to support the operator's movement along the direction of the rope. Experiments show that the portable rope-climbing robot can realize the functions of crossing, cable-stayed, vertical up and down multi-direction operation and rapid lifting in the high-altitude environment. At the same time, it shows good stability of high-altitude operation, with small size, light weight, high transmission efficiency, high timeliness, convenient and other advantages. It has important application value in earthquake rescue, special operation and robot transmission, and provides theoretical guidance and design basis for the research and development of rope-climbing robot.

Modeling friction and wear
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COUPLED ADHESION AND FRICTION OF GRAPHENE NANORIBBONS

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ABSTRACT

Peeling of graphene nanoribbons (GNRs) atop a graphene substrate can be used to characterize both adhesion and friction due to van der Waals interactions. In this work, we develop a continuum model for peeling and sliding of GNRs, using a periodic potential energy function to simulate the van der Waals interactions between the GNRs and the substrate in both the normal and tangential directions. Numerical simulations and associated analyses reveal remarkably rich dynamics in peeling and sliding of GNRs. It is found that the simple 90-degree peeling of a GNR depends primarily on the normal (adhesive) interactions, with negligible sliding or shear interactions. In contrast, peeling with the end fixed in the in-plane directions leads to stick-slip sliding, with a higher peeling force and a critical peeling angle depending on both adhesion and friction. Notably, the stick-slip sliding is facilitated by formation and gliding of strain solitons in GNRs, and different types of strain solitons may form in the zigzag, armchair and chiral GNRs. The peak pulling force as a measure of the sliding friction depends on the ribbon width quasi-linearly but becomes nearly independent of the ribbon length for relatively long GNRs (L >20 nm). Two cases with coupled peeling and sliding of GNRs are considered, and a simple analysis is proposed to simultaneously determine the adhesion and friction properties of GNRs from measurable quantities in potential experiments.

Machine learning methods for multiscale and multiphysics material modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STATISTICAL-PHYSICS-INFORMED NEURAL NETWORKS (STAT-PINNS): COARSE-GRAINING DISSIPATIVE EVOLUTION FROM PARTICLE DYNAMICS

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ABSTRACT

Physics-informed machine learning has become increasingly popular for discovering evolution equations from data. Such great success has led in the last few years to the development of thermodynamic-based approaches to enforce constraints, such as the second law of thermodynamics, and learn the thermodynamic structures of system, including the driving operators and potentials. Yet, unless further information is provided, the same macroscopic evolution can be obtained from different thermodynamic structures, indicating that this inverse learning problem is non-unique. This significantly challenges the discovery of the true physics. In this talk, we introduce a new machine learning strategy, called Statistical-Physics-Informed Neural Networks (Stat-PINNs), that can resolve this non-uniqueness issue for the first time, by encoding statistical mechanics relations. This strategy is developed for isothermal dissipative phenomena with the goal of predicting long-time macroscopic evolutions from short-time particle dynamics. Demonstrated on several examples, Stat-PINNs can successfully coarse-grain particle systems with known analytic macroscopic descriptions as well as discover, yet unknown, potentials and operators. Furthermore, our results indicate that the statistical mechanics relations within Stat-PINNs can increase the predictive capability and robustness of the machine learning algorithm.

Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADVANCED MATERIAL POINT FORMULATION FOR GEOMECHANICAL PROBLEMS UNDER EXTREME LOADING CONDITIONS

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ABSTRACT

The Material Point Method (MPM) has emerged as a valuable tool for modeling geomechanical phenomena like explosive mining or ground upheaval. Yet, it encounters significant challenges related to accuracy and pressure instability due to limitations in its domain integration scheme. Numerical issues, including undrained-induced pressure oscillation/locking and shock-induced instability under extreme loading conditions, further impede its effectiveness. This study introduces the VC-RKMPM approach [1], building upon previously developed variational consistent (VC) and reproducing kernel (RK) enhancements. The aim is to tackle these numerical challenges in geomechanical applications. Specifically, we implement a stabilized mixed formulation [2] to investigate blast behavior in porous geomaterials. Our approach involves exploring suitable stabilization techniques for shock wave dynamics and integrating a pressure stabilization method to rectify the shortcomings of the equal order approximation scheme. To demonstrate the efficacy of our proposed framework, we present several benchmark numerical examples. These examples showcase how our approach effectively addresses the aforementioned issues, thereby enhancing the reliability and accuracy of geomechanical simulations.

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The phase field method for fracture: Theory, numerics, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A PHASE FIELD MODEL FOR FATIGUE FRACTURE CONSIDERING CRACK RETARDATION EFFECT DUE TO SINGLE OVERLOAD

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ABSTRACT

Phase Field Method is a powerful tool which takes the advantages of fracture mechanics and continuum damage mechanics [1-3]. Over the last decade, the phase field method has been developed to simulate the brittle fracture, ductile fracture, cohesive fracture, and fracture in multi-physics problems. It has the potential capability to model complicated crack patterns including crack initiation, crack propagation, crack merging, crack branching and crack kinking. In this work, a phase field fatigue model is proposed to simulate fatigue crack propagation behavior considering crack retardation effect based on the Griffith threshold degradation method and the Wheeler model.

Based on the Griffith threshold degradation method, the crack tip fatigue degradation zone is defined and the analytical solution of fatigue crack growth rate can be derived. This method is combined with the phase field model and fatigue acceleration algorithm. The simulation results show that the fatigue crack growth rate obtained by the phase field model of AT1 dissipation function is more consistent with the analytical solution. The fatigue life increases with the decrease of the radius of fatigue degradation zone. Compared with the other numerical methods, the proposed phase field fatigue model requires fewer parameters, and the simulation results are closer to the experimental results.

Based on the Wheeler model for crack growth retardation, we proposed a three-parameter driven degradation function for phase field fatigue model that responds to fatigue crack propagation retardation induced by single overload. This modified phase field fatigue model high load history variables is demonstrated to effectively capture the whole stage of fatigue crack retardation (including: delayed retardation, nonlinear recovery, retardation vanish). Simulation results are also in good agreement with the experimental results.

The predictions of the proposed model agree well with the experimental results reported in the literature. This achievement contributes significantly to the structural safety design and life prediction, and can provide a theoretical basis for structural integrity assessment.

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Computational fluid dynamics (CFD) and fluid-structure interaction (CFSI): Methods and Applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

WEAKLY ENFORCED DIRICHLET BOUNDARY CONDITION IN HEMODYNAMIC SIMULATIONS

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ABSTRACT

It is well-known that the weak enforcement of the Dirichlet boundary condition can be effective in the wall modeling of turbulent flows [1]. Current research assesses the wall-modeled computation results with DNS or experimental data based on relatively simple geometries (such as channel flow). It is less common to see studies that considered weak enforcement of boundary conditions in cardiovascular flows. Blood flows may involve complex flow patterns, including laminar, transitional, and fully turbulent flows. This demands a specific consideration of the wall modeling. Moreover, the geometry of patient-specific models involves tortuous paths, bifurcating branches, and non-uniform vessel radius. Consequently, the boundary layer mesh generation for blood flows can sometimes be quite challenging. Thus, it remains a crucial task to evaluate the existing treatment of the wall boundary and offer guidance in cardiovascular applications.

In this study, we investigate the effect of the weakly enforced no-slip boundary condition of the incompressible Navier-Stokes equations in hemodynamic simulations. Our scheme is based on the residual-based variational multiscale method and the generalized-α time marching method. Three approaches are studied: (i) strong enforcement for the velocity in all directions with boundary layer meshes, (ii) weak enforcement for the velocity in all directions, (iii) weak enforcement for the wall-tangential velocity component in combination with strong enforcement for the wall-normal velocity component. Besides, we will discuss a critical method for generating outward normals at the nodes on polygonal surface meshes [2]. The nodal normals are employed in the third approach, and they can be applicable for postprocessing wall shear stresses.

The adopted numerical benchmarks include (i) the idealized medical device designed by the US Food and Drug Administration (FDA), (ii) the centrifugal blood pump designed by the FDA, (iii) CFD and FSI cases of the aorta, with emphasis on physiologically realistic domains. We will compare our results to experimental data and existing numerical results, and we will then draw conclusions based on the assessment.

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MATHEMATICS-INFORMED NEURAL NETWORK FOR WAVE SCATTERING PROBLEMS

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ABSTRACT

In this work, we propose a mathematics-informed neural network (MINN) approach for resolving the long-term challenge in wave scattering modelling. The key contribution is the innovative concept of the incorporation of the Cauchy-Riemann equation into machine learning architectures, which eventually learn to produce matrix kernel factorization for Wiener-Hopf analytical models. To validate and demonstrate the approach, a guiding example of wave scattering from parallel hard-soft plates is studied by comparing the machine learning results with the available analytical solutions. Overall, the proposed MINN approach could extensively enhance the theoretical modelling capability for a number of wave scattering and fluid mechanics problems.
The code can be found at: https://github.com/lscapku/MINN.

Biomechanics of hard tissues: From experiments and simulations to clinical applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFECTS OF THE LIGAMENTS ON VERTEBRAE AND MATERIAL PROPERTIES OF DISCS DURING THE S2AI SURGERY FOR SCOLIOSIS: A FINITE ELEMENT STUDY

Ying-Hsuan Huang[*1], Chaung-Sian Yang[1], Chi-Kuang Feng[2], Jing-Jing Fang[1] and Chung-De Chen[1]*

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ABSTRACT

Scoliosis and anterior pelvic tilt are frequently observed spinal deformities that can significantly impact a patient's quality of life and overall health. Early diagnosis and treatment are essential for correcting these deformities. Traditionally, clinical observations, radiology, and surgeries have been relied upon for research in the field of scoliosis and pelvic tilt, but these methods have limitations. Finite element method (FEM) has received attentions as a computational method to study spinal models, enhancing our understanding of biomechanical behaviors.

The objective of this study to simulate the procedure of a scoliosis correction surgery with S2AI by using FEM. The numerical model to simulate the entire correction surgery process, providing useful insights that can guide improvements in surgical procedures. The geometric models are established based on Computed Tomography (CT) data obtained from a 16-year-old female patient. The finite element model was conducted with the commercial FEM software ABAQUS. The model is composed of lumbar L1 to L5, sacrum, pelvis, ligaments, discs, screws (including S2AI) and rods. The discs and ligaments are modeled by hyperelastic material and spring elements, while the others are by linear elastic materials. The acetabulum is fixed for boundary condition. The analysis for the surgical procedure includes four stages: the establishment of follower load, movement of screws and vertebrae, contact between screws and rods, and the release of screws. The effects of the ligaments on vertebrae and material properties of discs during the S2AI surgery for scoliosis are investigated by FEM.

According to the FEM results, a spring back is observed in the finite element calculations after rod release. It reveals that the rod near S2AI have lowest spring back displacement as it is near fixation region. The spring back displacements increases for upper vertebrae. The existence of spring back displacements suggests that the correction angle may be less than expected. The pullout forces of screws can also be calculated by the FEM model. The risk for screw-loosening can be evaluated.
The numerical results obtained in the model can provide a reference to a doctor for plan of pre-operation.

Fracture, damage and failure mechanics of cementitious materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTI-SCALE DAMAGE AND FRACTURE SIMULATIONS OF CONCRETE

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ABSTRACT

Concrete is composed of multiple phases such as coarse aggregates, mortar, pores, initial cracks, and interfaces at micro/meso-scale, which exhibit randomness, heterogeneity and phasic interactions contributing to highly nonlinear and stochastic failure processes at material/structural level. Accurately and efficiently simulating the multi-scale damage and fracture of concrete has become one of the major challenges in the fields of composites science and computational mechanics. This paper introduces our recent studies on micro-CT experiments and static/dynamic fracture simulations of concrete, including the generation of high-fidelity random fields and novel models with realistic aggregate morphology and distribution. We also present automatic meshing algorithms for complex meso-structures integrated with the Scaled Boundary Finite Element Method (SBFEM) and Smoothed Finite Element Method (SFEM), and develop efficient computational frameworks with the discrete cohesive model [1], quasi-brittle phase field model [2], and nonlocal damage model [3], respectively. Through a series of typical benchmarks, the work validates the simulated fracture processes and load-carrying capacities, evaluates the accuracy and computational efficiency of various algorithms, and offers flexible control in reconstructing meso-structures. We focus on the crack-netting mechanisms, stochastic mechanical responses, and impacts of meso-scale parameters on macroscopic performance, elucidating the complicated multiple micro-crack initiation, propagation, branching, merging, and macroscopic crack formation. The proposed computational frameworks are also applicable to other composite materials such as fiber-reinforced composites, metal-matrix composites and ceramic-matrix composites, benefiting the development of new materials and structures.

Keywords
Damage and fracture simulations; mesoscale concrete; quasi-brittle phase field model; random fields; micro-CT image-based modelling

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Multiscale modeling, analysis and numerical methods of material defect and inhomogeneities
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NUMERICAL STUDY FOR SHEAR-INDUCED AMORPHIZATION IN ALLOY

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ABSTRACT

Amorphization due to severe plastic deformation has been discovered in various crystalline materials. Despite its importance, developing a rigorous and general theory of strain-induced amorphization remains a significant challenge due to the intricate nature of modeling microstructural changes and deformation mechanisms. In this study, we propose a novel model integrated with elastic-plastic theory to shed light on shear-induced amorphization in nanocrystalline alloys. Our model incorporates the martensite transformation of the austenite phase under large plastic deformation, followed by the intensification of crystal fracture on the martensite phase to form an amorphous phase. Our simulations suggest that amorphous nucleation is more likely to occur in high-stress regions, such as shear bands, and that the critical plastic strain for amorphization increases as grain size grows. These observations align with experimental data, indicating that our phase-field model captures the physical picture of shear-induced amorphization and can predict the threshold for amorphization. Overall, our work offers valuable insights into shear-induced amorphization and paves the way for enhancing the understanding of amorphous materials and fostering the development of more precise and comprehensive models for investigation.

Phase-field interface modeling for multiphase and multiphysics simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CONSISTENT AND CONSERVATIVE PHASE-FIELD METHOD FOR CHALLENGING INCOMPRESSIBLE AND COMPRESSIBLE MULTIPHASE PROBLEMS

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ABSTRACT

The Phase-Field method has been widely used to model complex systems including moving and deforming interfaces, as either a thermodynamic model or numerical tool. However, the coupling of the Phase-Field description of interfaces to the dynamics of continua is non-trivial and missed in the literature. This presentation provides an overview and recent progress on the consistent and conservative Phase-Field method, which addresses the coupling of the Phase-Field mechanism to a wide range of challenging multiphase problems including an arbitrary number of materials, arbitrarily large density ratios, heat and mass transfer, solidification and melting, and shock and rarefaction waves. The corresponding numerical framework that preserves the physical structure of both incompressible and compressible multiphase flows is also introduced. Various multiphase problems are reported to demonstrate the efficacy of the Phase-Field method.

Buckling analysis and design of thin-walled structures based on novel and intelligent computational methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODEL-REDUCED IGA BASED ON LOCALLY-REFINED SPLINES FOR BUCKLING ANALYSIS OF IMPERFECT FGM SHELLS

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ABSTRACT

Buckling responses of imperfect FGM shells (perforated or cracked), whose material properties grade continuously in specified directions, are numerically investigated through the combination of extended isogeometric analysis and isogeometric finite cell method based on locally-refined splines. On the basis of inheriting the superiorities of the geometric smoothness and exactness of isogeometric analysis, the locally-refined splines can accurately describe the geometry of the middle-surface of FGM shells and flexibly control the meshes' density around the defects, directly linking the CAD model to the structural one. Besides, the higher continuity of locally-refined splines basis functions can automatically satisfy the requirement of C1-continuity for the Kirchhoff–Love theory. The main superiority of the presented method is that the representation of all types of internal defects is mesh-independent of the underlying grids. The displacement discontinuous across the crack face and the stress singular phenomena in the vicinity of the crack tip are efficiently captured by using the local enrichment patterns in isogeometric approximation. The geometric interfaces of cutouts are approached and approximated by means of an adaptive integration scheme based on quadtree subdivision technique in the distinguished cut elements. This implementation avoids the tricky process of multiple patches to represent the geometry of shells, thus eliminating the enforcement of higher continuity across these patches' boundaries. The cylinder arc-length iteration technique in combination with modified Newton–Raphson iteration algorithm, which embeds three strategies arc-length control, eigenvalue analysis and mode imperfections, is applied to implement geometrically nonlinear dynamic analysis. Furthermore, to maintain a balance between computational efficiency and computational accuracy, the reduced-order modeling technique via proper matrix decomposition is employed into the isogeometric framework coupled with dynamic response analysis. After validating the effectiveness and reliability of the developed approach through available benchmark problems, a series of factors, including material volume fraction, boundary condition, defects size, imperfection sensitivity etc., affecting the buckling responses of imperfect FGM shells are performed and investigated.

Design beyond optimization: Why, what if, and how much?
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ASYMPTOTIC DESIGNABILITY AND THE STRUCTURE OF SELF-ASSEMBLY

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ABSTRACT

The spontaneous self assembly of complex structures from simple building blocks is of prime importance in biology and is a promising candidate for the creation of novel functional materials. The potential for synthetic material design leads directly to a formulation of self assembly as an inverse problem: “How should we tune our building blocks, such that they self-assemble into the structures or materials we desire?” However, such inverse problems are usually tackled through direct optimization, which can lead to one-off solutions that do not generalize or reveal broader principles.
Here, we will show that the space of self-assembly yields has an internal structure that is hierarchically organized. To achieve this, we exploit an underlying correspondence between inverse self-assembly and the theory of convex polyhedra. We then introduce the concept of Asymptotic Designability, which refers to a structure (or group of structures) that can, in principle, be assembled at high yield. Using algorithms from polyhedral computation, we can completely and efficiently enumerate all sets of asymptotically designable structures, which form the basis for a comprehensive view of the design space. Furthermore, in an asymptotic regime of parameter space, the mapping from parameters to yields becomes linear, meaning that the complete inverse problem reduces to an easily solvable linear program. This framework is highly generalizable, provides geometrical intuition for complex self assembly processes, and can easily incorporate experimental constraints.

Enabling technologies for digital twins: Model reduction and scientific machine learning
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SURROGATE MODELS FOR STROKE OPTIMIZATION IN PARAMETERIZED FLOWS

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ABSTRACT

Simulating complex flow systems with parameterized geometries in order to determine critical quantities of interest (QoI) is often prohibitively expensive due to the high dimensionality of the problem. This challenge is further inescapable in optimization loops where multi-querying is essential to the scheme. Additionally, simplified models usually lack the accuracy needed by physicists and engineers to provide reliable QoI estimates. This computational bottleneck poses a significant challenge for the effective conception, design, and operation of industrial systems, especially when geometric parameters are involved.

After providing a brief overview of a priori and a posteriori ROM strategies for geometrically parametrized incompressible flows [1], optimal strokes for the push-me-pull-you (PMPY) model of an euglenoid micro-swimmer are determined using the non-intrusive Encapsulated Proper Generalized Decomposition (PGD) to calculate separated expressions of forces and velocity, explicitly depending on the design parameters [2].

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Computational models and methods for predicting cancer progression and treatment response
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PATIENT-SPECIFIC, ORGAN-SCALE PREDICTION OF PROSTATE CANCER GROWTH AND CLINICAL PROGRESSION DURING ACTIVE SURVEILLANCE

Guillermo Lorenzo[12], Chengyue Wu[32], Joshua P. Yung[3], John F. Ward[3], Hector Gomez[4], Alessandro Reali[5], Thomas Yankeelov[23], Aradhana M. Venkatesan[3] and Thomas J.R. Hughes[2]*

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ABSTRACT

Active surveillance (AS) is a standard clinical management option for the abundant newly-diagnosed prostate cancer (PCa) cases exhibiting low and favorable intermediate clinical risk. Since these tumors do not require immediate treatment, AS offers longitudinal monitoring via multiparametric magnetic resonance imaging (mpMRI), serum prostate-specific antigen (PSA) tests, and biopsies. If these exams detect progression to higher-risk disease, then the patient is prescribed treatment. Hence, AS combats the current overtreatment of PCa. However, AS is based on an observational population-based approach, which does not account for each patient's tumor dynamics and may delay the detection of tumor progression. This work proposes to address these issues by means of personalized predictions of PCa growth and progression informed by each patient's clinical and mpMRI data collected during AS [1]. We use a biomechanistic model to describe spatiotemporal PCa growth in terms of tumor cell density as a combination of tumor cell mobility and net proliferation. This model is posed on the patient's prostate geometry defined on T2-weighted MRI data. Apparent diffusion coefficient (ADC) maps obtained from diffusion-weighted MRI data are used to estimate tumor cell density. Model calibration consists of minimizing the mismatch between model predictions and mpMRI measurements of tumor cell density, and we validate predictions against further mpMRI measurements at later times. We leverage isogeometric analysis to solve our model numerically and, hence, obtain patient-specific tumor forecasts. Additionally, we construct a logistic classifier of PCa risk utilizing model-based biomarkers calculated from the model forecasts (e.g., tumor volume, total proliferation activity) at the times of histopathological assessment (i.e., biopsy, surgery). In a cohort of 16 PCa cases with three longitudinal mpMRI datasets, we obtained a concordance correlation coefficient (CCC) for tumor volume of 0.89 both at the second and third scan times (i.e., calibration and prediction horizons). The corresponding spatial fits and forecasts of tumor cell density maps resulted in a CCC of 0.59 and 0.60, respectively. Our logistic classifier of clinical risk yielded an area under the receiver operating characteristic curve of 0.90, operates at optimal sensitivity, specificity, and accuracy of 86.7%, 93.8%, and 90.3%, and anticipates PCa progression by more than 1 year with respect to standard AS. Thus, we believe that our technology shows promise to guide clinical decisions for each PCa patient during AS.

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Predictive digital twins
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

WALKING PARAMETER INFERENCE FROM STRAIN DATA FOR A FOOTBRIDGE

Adrian Humphry[*1], Akmal Bakar[1], Jenmy Zhang[1], Farhad Javid[1], Patrick Nadeau[1], Mehran Ebrahimi[1], Adrian Butscher[1], Alex Tessier[1], Jesus Rodriguez[1], Marie-Jo Azzi[2] and Charbel Farhat[2]*

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ABSTRACT

Accurate identification of structural loads is critical in digital twin applications such as structural health monitoring. Structures are rarely equipped with sensors that can adequately characterize the loads but may have sensors that measure the resulting response. In this work, we consider an indoor footbridge monitored by six strain gauges. We demonstrate that we can infer from strain data a detailed description of a pedestrian's motion, including speed, stepping rate and walking path. We observe that the walking path has a significant impact on structural response. Furthermore, we observe that a higher fidelity walking path model (e.g. allowing for curved walking paths) improves our ability to infer other parameters of the pedestrian motion. The increased fidelity in the walking model incurs an increased computational cost to our parameter inference procedure, motivating the following contributions.

Our first contribution is the development of a projection-based reduced order model (pROM) for the bridge which ensures rapid evaluation of the strain and its gradient with respect to the walking model parameters. In standard pROM training, we collect snapshots of the system response for representative load conditions and then construct the reduced model using the snapshots. However, the standard sampling procedure is intractable in our case because an attempt to sample the space of all possible bridge traversals results in too large of a training set. Instead, we exploit that the walking load is decomposable into individual footfall loads and develop a pROM training procedure that takes advantage of such a decomposition.

Our second contribution is a tailored optimization strategy that identifies the walking model parameters, enabling the use of a walking model with sufficient fidelity to accurately describe complex pedestrian motion. We find the pedestrian motion that minimizes the difference between the measured strain and the predicted strain, leveraging the speed-up provided by the pROM and employing a gradient descent method with a modified basin-hopping scheme to quickly minimize this difference. We apply these methods to strain data collected from a real bridge and find that our preliminary results agree well with camera footage of the actual pedestrian motions.

Microstructures of chemically complex materials and their impacts on material properties from multiscale simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MECHANICAL INSIGHTS THROUGH MULTI-SCALE SIMULATION OF CHEMICALLY COMPLEX INTERFACES IN ALL-SOLID-STATE BATTERIES

Ming-Yuan Hung[1], Yu-Ting Tai[1], Hong-Zong Huang[1], Yueh-An Wu[1] and Hong-Kang Tian[1]*

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ABSTRACT

All-solid-state batteries are at the forefront of energy storage innovation, offering heightened safety and reliability. This research delves into the intricate world of chemically complex materials, specifically focusing on the electrode-electrolyte interface. Challenges at this interface, leading to high impedance and chemical interphases, pose critical questions regarding their impact on battery performance. Drawing inspiration from the chemically complex materials paradigm, we present a study employing Density Functional Theory (DFT) and Finite Element Analysis (FEA) to unravel the microstructural nuances of the $LiCoO_2$ (LCO) /$Li_{1+x}Al_xTi_{2-x}(PO_4)_3$ (LATP) interface. Co-diffusion into LATP and Co_3O_4 formation during sintering have been identified as key processes. Our investigation screens the most energetically favorable LATP atomic structures, replacing Ti with Co (LACTP). Through a continuum model integrating DFT-calculated properties, we simulate the mechanical response, uncovering crucial insights into material properties. Utilizing a particle-based 2D composite-electrode geometry, grounded in scanning transmission electron microscopy and electron energy-loss spectroscopy (STEM-EELS) images[1], we bridge DFT and FEA simulations. This approach not only allows us to understand stress generation near the interfaces during LCO lithiation but also provides a comprehensive view of the microstructure. DFT calculations highlight a 12.25 GPa decrease in Young's modulus when LATP transforms into LACTP and a transformation into Co_3O_4 results in a 77.89 GPa increase in Young's modulus with a 0.053 increase in Poisson's ratio compared to LATP. Integrating these insights, FEA simulations revealed that Co diffusion significantly increases peak stress within the LATP, escalating from 2966 MPa to 5650 MPa, potentially leading to crack formations, emphasizing the importance of microstructure in battery performance. This study contributes to the symposium's focus by utilizing computational techniques to explore chemically complex materials' microstructures, offering valuable insights into the intricate relationships among process, structure, and properties, thereby enhancing our understanding of both material composition and their applications in energy storage.

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Uncertainty quantification and reliability analysis in engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

UNCERTAINTY QUANTIFICATION OF STOCHASTIC FUNCTIONALLY GRADED PLATE STRUCTURES BASED ON NOVEL PROBABILITY INTEGRAL PERSPECTIVE

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ABSTRACT

The functionally graded plate structures with excellent thermal resistance and high efficiency of load-bearing capacity have a broad application prospect in various engineering fields. Determining the responses' probability density functions (PDFs) and dynamic reliabilities of stochastic functionally graded plates subjected to random excitation is of great significance in the field of uncertainty quantification and structural design, while the popular intrusive stochastic finite element methods (SFEMs) are difficult for solving this complex problem. The direct probability integral method (DPIM) was recently developed by the authors' team to calculate the response PDFs and reliabilities for stochastic structures. For the functionally graded plates considering random fields of structural parameters and external random excitations, this paper proposes an efficient and accurate non-intrusive SFEM based on the novel perspective of probability integral. Firstly, the probability density integral equation (PDIE) is derived based on the principle of probability conservation, and the DPIM with adaptive strategy is introduced from the viewpoint of probability integral. Secondly, decoupling the deterministic finite element analysis and PDIE, the non-intrusive approach based on DPIM is constructed to compute the PDFs of random vibration responses and dynamic reliabilities of functionally graded plates, where the representation of random field is implemented through Karhunen-Loève expansion, and the random excitation is generated by the random function-based spectral representation. Then, the comparisons of the results with those from Monte Carlo simulation and the literature indicate the high accuracy and efficiency of the proposed non-intrusive method. Finally, the key parameters affecting the nonlinear random vibration responses of stochastic functionally graded plates are elaborated. This study possesses has important scientific significance and application potential for uncertainty quantification, reliability and safety assessment of functionally graded plate structures.

Modeling and simulation of the electro-chemo-thermo-mechanical interactions in energy transition and energy storage systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ELECTROCHEMICAL RESPONSES IN FOCUS: A VOLTAMMETRIC EXPLORATION OF TWO-PHASE LITHIATION IN HIGH-CAPACITY ANODES

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ABSTRACT

The increasing demand for higher energy capacity in lithium-ion batteries has underscored the significance of modeling lithiation with alternative electrode materials, such as silicon (Si) and tin (Sn). This research addresses the need for comprehensive insights into the (dis)charging process, particularly focusing on the intricate phase transformations in the anode. Phase-field modeling has proven effective in capturing these transformations [2], revealing volumetric deformations of up to 300% during (dis)charging cycles [1]. Unfortunately, these deformations compromise material integrity, leading to reduced battery cycle life and reliability.

To address these challenges, our work presents a novel framework for modeling lithiation in materials exhibiting two-phase diffusion using phase field modeling. Unlike previous models limited to single-phase diffusion, our framework provides a more realistic representation of the diffusion process. This realism is achieved by incorporating the time-dependent voltage applied to the anode, a crucial factor in understanding the electrochemical response during lithiation [3].

Furthermore, we leverage the currents generated during the lithiation and delithiation processes to conduct a comprehensive voltammetric study. This study goes beyond existing research by considering the impact of phase separation on the currents developed during Li-ion battery operation. Our findings aim to contribute valuable insights into optimizing battery performance and addressing challenges associated with phase transformations, ultimately advancing the development of high-capacity anodes for lithium-ion batteries.

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Design beyond optimization: Why, what if, and how much?
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PATH PLANNING IN A DYNAMIC ENVIRONMENT USING SPHERICAL PARTICLE SWARM

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ABSTRACT

Efficiently planning an Unmanned Aerial Vehicle (UAV) path is crucial, especially in dynamic settings where potential threats are prevalent. A Dynamic Path Planner (DPP) for UAV using the Spherical Vector based Particle Swarm Optimization (SPSO) technique is proposed in this study. The UAV is supposed to go from a starting point to an end point through an optimal path according to some flight criteria. Path length, Safety, Attitude and Path Smoothness are all taken into account upon deciding how an optimal path should be. The path is constructed as a set of way-points that stands as re-planning checkpoints. At each pathway-point, threats are allowed some constrained random motion, where their exact positions are updated and fed to the SPSO-solver. Four test scenarios are carried out using real digital elevation models. Each test gives different priorities to path length and safety, in order to show how well the SPSO-DPP is capable of generating a safe yet efficient path segments. Finally, a comparison is made to reveal the persistent overall superior performance of the SPSO, in a dynamic environment, over both the Particle Swarm Optimization (PSO) and the Genetic Algorithm (GA). SPSO outperformed both PSO and GA, showcasing cost reductions ranging from 330% to 675% compared to both algorithms.
In essence, this work focuses on:
1) Introducing Spherical Particle Swarm Optimization Dynamic Path Planner (SPSO-DPP).
2) Investigating the efficiency of SPSO-solver within a dynamic setting characterized by the presence of randomly moving obstacles.
3) Comparing the SPSO-DPP performance with PSO and GA performances in a dynamic environment.
Four scenarios have been presented, each of which modifies the parameters to reduce distance or prioritize safety. The results demonstrate that SPSO consistently produces superior cost values than both GA and PSO, demonstrating the algorithm’s efficacy in generating optimal paths. The effect of prioritizing distance reduction above hazard avoidance is best shown in Case 3, where the decision leads to a more direct path that circumvents obstacle constraints. This realization emphasizes the necessity of carefully weighing objectives against constraints in situations including dynamic UAV path planning. Furthermore, we intend to validate our algorithm’s output with real-world simulations, to confirm that the algorithm operates as efficiently and robustly as possible under demanding and dynamic UAV conditions.

Geomechanics of the cryosphere
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

OBSERVATIONAL GUIDANCE FOR MECHANICAL MODELS OF PACK ICE

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ABSTRACT

Past studies find there is multi-fractal behavior for horizontal sea-ice deformation from 10 to 1000 km. Various observational studies point to seasonality and large inter-annual variability in this scaling behavior, suggesting different mechanical energy dissipation rates based on the state of the ice pack. Moreover, recent field observations demonstrate that such behavior does not hold for spatial scales below 10 km}. Indeed, we find that sea-ice deformation is not scale invariant between the scale of individual sea-ice floes and aggregates of floes. Therefore, we cannot expect the same physical laws to describe sea-ice mechanics over these regimes, or the forcing and boundary conditions must be treated differently at different scales. Using an assumed scaling behavior as a metric to validate models that resolve sea ice floes and their interactions is thus not recommended. However, observations might provide insight into the different physical regimes of pack-ice mechanics allowing, in turn, better models to be designed that capture seasonality and the mechanical response to ice-pack state changes, such as increasing damage, realistically. We will present a summary of current knowledge on multi-scale behavior of sea ice, describing the features that define each scale over which a single model can be applied and the bounds defining these scales.

Imaging and computational methods for biomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PRECONDITIONED SOLVERS FOR COMPOSITE DG DISCRETIZATIONS OF CARDIAC CELL-BY-CELL MODELS

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ABSTRACT

The drive to better understand complex phenomena like cardiac functions has led to mathematical models that are able to describe the multiscale structure and dynamics of the heart. The numerical simulation of these complex cardiac models is very challenging since it requires high-resolution space and time discretizations, as well as numerical tools that can handle natural discontinuities (for instance, disconnected cells).

The development of effective and scalable solvers for the solution of these models has grown increasingly in the last decade, and modern computational architectures have increased the possibility to run large-scale simulations within reasonable computational times. In any case, the multiscale systems arising from discretizations of such models has required the development of specific techniques which can balance accuracy in the solution while being computationally competitive (in terms of efficiency and scalability). Indeed, being able to describe and computationally reproduce the many interactions between the macroscopic and microscopic events leads to numerical choices that yield large scale nonlinear algebraic systems of equations, exceeding millions of degrees of freedom.

In this talk, we focus on the numerical simulation of the cardiac electrical activity from a microscopic point of view, by means of cell-by-cell mathematical models. We propose ad-hoc preconditioned solvers inspired by well-known Domain Decomposition methods, e.g. the generalized Drijia-Smith-Widlund (GDSW) or non-overlapping Spectral Additive Schwarz (NOSAS), where special constraints are imposed in order to reflect the physiological discontinuities of the mathematical model. We provide a strong theoretical analysis, validated then through extensive numerical tests, showing scalability and quasi-optimality of these solvers. These results provide a basis for improving parallel solvers for cardiac electrophysiology models that combine parallel efficiency and solution accuracy.

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Imaging and computational methods for biomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREDICTING LIVER FIBROSIS STAGES: A HYBRID APPROACH INTEGRATING MACHINE LEARNING AND DATA-DRIVEN COMPUTATIONAL TECHNIQUES WITH DCI-MRI

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ABSTRACT

Liver diseases consistently rank among the top ten causes of death in numerous countries. The progression of these diseases is generally categorized into three stages: liver fibrosis, liver cirrhosis, and liver cancer. Addressing the need for early diagnosis and intervention, a research study focusing on clinical practice is underway, developing noninvasive techniques to determine liver disease status. Early detection of liver fibrosis, coupled with appropriate treatments, can significantly reduce the risk of hepatocellular carcinoma. We propose a hybrid approach that integrates machine learning methods with a data-driven computational technique employing dynamic contrast-enhanced MRI (DCI-MRI) for predicting a patient's fibrous stages, healthy, mild, and severe. The kernel component of the computational technique is a Darcy solver weakly coupled with an unsteady convection-diffusion solver that is used for simulating the blood flows through the liver, assumedly as a kind of porous medium, and the relative signal enhancement scanned by MRI varied in time. During the preprocessing phase, we extract new features simulating liver properties, including porosity, diffusion rate, and flow speeds of the portal vein and hepatic artery. Combining these features with patients' blood tests and the characteristics of DCE-MRI curves, we used KNN and Naive Bayes models in conjunction with feature selection to achieve the accuracy of predicted results of healthy versus others and severe versus others around 80%. This study underscores the potential value of simulating liver signal concentration models in liver fibrosis assessment, providing biomedical researchers with a deeper understanding and new avenues for research.

Advanced computational mechanics based on data-driven techniques for structure, structural dynamics and aeroelasticity
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATION OF THE TWO-LEVEL HYPER-REDUCTION APPROACH FOR THE MULTI-BODY CONTACT-IMPACT SIMULATION

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ABSTRACT

Multi-body contact analysis will become computationally cumbersome for a complex object usually due to large number of degrees of freedom and nonlinearities involved. Therefore, the reduced order model (ROM) will be used for an efficient alternate computation. Projection-based ROM (PROM) will be a popular method that reduces the order by projecting the governing formulation. Meanwhile, a contact analysis with enhanced computational capability is often applied with an explicit method to extract the result at a short time step. In such circumstance, however, there is a limitation of the reducing time step size with a sole PROM due to repetitive matrix-vector multiplication for the projection. Therefore, it is additionally required to apply a hyper-reduction method that improves the computational time-saving capability of PROM by employing only sampled indices.

In this presentation, both PROM and hyper-reduction approach will be incorporated into the three-dimensional multi-body contact analysis. The proper orthogonal decomposition (POD) idea is used for reducing the order of the matrices. Also, the energy-conserving sampling and weighting method [1] is applied to select a dominant element in the contact-impact response to reduce the cost of element-wise computation of nonlinear force vector. The velocities of the multiple bodies are selected as the parameter. The discrete empirical interpolation method [2] will also be attempted to reduce the computational cost of the contact force.

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HYBRID STRESS AND HEAT-FLUX FORMULATION OF THERMODYNAMICS FOR LONG-TERM SIMULATIONS IN THERMO-VISCOPLASTICITY

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ABSTRACT

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We present a variational formulation for coupled problems in thermodynamics the most suitable for long-term simulations of plastic behavior. We start with mixed formulation that is first regularized, which allows us to eliminate the rotation field and recover the corresponding hybrid stress format for equations of motion and transient heat conduction. The regularized variational formulation is further combined with discrete approximation based upon the Raviart-Thomas vector space for both mechanical and thermal fields, which enforces continuity across element boundaries for stress vector and normal component of heat flux. The conservation properties are validated with energy-conserving scheme for thermoelastic behavior. The time integration of thermo-viscoplastic behavior is carried out by energy-decaying scheme to provide superior accuracy for computed stress in a long term simulation. The proposed approach offers higher computational robustness and results accuracy than the classical finite elements and time-integration schemes. Such a performance is illustrated on several numerical simulations in non-stationary problems for thermo-viscoplastic behavior.

A MULTISCALE METHOD TO SOLVE PARTICLE-LADEN TURBULENT FLUID FLOWS

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ABSTRACT

Particle-laden flows refer to a kind of two-phase fluid flow in which one of the phases is continuously connected and the other phase is made up of small immiscible particles. A wide variety of scientific and engineering applications belong to particles-laden flows, for instance dispersion of contamination in the atmosphere, fluidization in combustion processes, deposition of aerosols in aerosol drugs, spread of virus in the air, rain formation in clouds, sand and dust storms, protoplanetary disks, volcanic eruptions, geological sedimentation processes, pharmaceutical sprays, liquid-fuelled combustion and solid rocket motors, among many others.

Typically, the fluid is treated in a Eulerian frame, while the particles are treated in a Lagrangian way. However, problem with the Lagrangian treatment of the particles is that once the number becomes large, it may require a prohibitive amount of computational power to track a sufficiently large sample of particles required. In addition, if the particles are sufficiently light, they behave essentially like a second fluid. This is the main objective of this presentation.

On the other hand, due to the interactions between turbulence structure and dispersed particles, turbulence characteristics of momentum and heat transport can be modified by the presence of particles. This last phenomenon is known as turbulence modulation and can lead to a significant increase or decrease in the parameters that regulate turbulence.

The authors presented in Ref. [1] a multi-scale method called Pseudo-Direct Numerical Simulation (P-DNS) [2] to study the phenomenon of turbulence modulation in a particle-laden flows. However, in that article, the particles in both, the fine scale and the coarse scale, were treated in a discrete way moving in a Lagrangian reference frame within the fluid. In this presentation, the same P-DNS method will be used to simulate the presence of particles as a continuum function that moves within the fluid. In this way, the need to represent each of the particles that move in the fluid is avoided.

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Advances in numerical methods for solution of PDEs
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

OPTIMAL LOCAL TRUNCATION ERROR METHOD FOR SOLUTION OF PDES ON IRREGULAR DOMAINS AND INTERFACES WITH OPTIMAL ACCURACY AND UNFITTED CARTESIAN MESHES. COMPARISON WITH FINITE ELEMENTS.

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ABSTRACT

Here, we review as well as present some new developments of the optimal local truncation error method (OLTEM) for the solution of partial differential equations [1]. Similar to the finite difference method, the structure and the width of discrete equations are assumed in advance. The unknown coefficients of the discrete system are calculated by the minimization of the local truncation error. The main advantages of OLTEM are an optimal high accuracy of discrete equations and the simplicity of the formation of a discrete (semi-discrete) system for irregular domains and interfaces (composite materials). In contrast to finite elements, trivial unfitted Cartesian meshes (no need in complicated mesh generators) are used with OLTEM. OLTEM does not include unknowns on irregular boundaries and interfaces. The known interface and boundary conditions at small number of selected points are added to the discrete equations as the right-hand side. A new OLTEM post-processing procedure for the calculation of the spatial derivatives of the primary functions (e.g., stresses or heat fluxes) that is based on the use of original PDEs significantly increases the accuracy of the spatial derivatives. For example, we have obtained the 10-th order of accuracy for stresses calculated by OLTEM with ‘quadratic elements’ applied to elastostatics problems with heterogeneous materials and irregular interfaces. Currently, OLTEM has been applied to the solution of the wave, heat, elastodynamics, Helmholtz, Poisson, Stoke’s and elastostatics equations. The theoretical and numerical results show that at the computational costs of linear finite elements, OLTEM yields the 4th order of accuracy for the considered scalar PDEs on irregular domains (it is much more accurate compared with linear and high-order finite elements at the same number of degrees of freedom). E.g., 3-D numerical examples on irregular domains show that at accuracy of 5%, OLTEM applied to the wave equation reduces the number of degrees of freedom by a factor of greater than 1000 compared to that for linear finite elements. At the computational costs of quadratic finite elements, OLTEM yields the 10th order of accuracy for the time-independent elasticity equations and the 11th order of accuracy for the Poisson equation with complex irregular interfaces [1], i.e., the increase in accuracy by 7 and 8 orders compared to FEM.

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LARGE-SCALE FLUID SIMULATIONS OF SUSPENSION OF DEFORMABLE CAPSULES IN TOROIDAL TUBE

Satoshi Ii[1], Kazuyasu Sugiyama[2], Shigeho Noda[3], Takeharu Matsuda[1] and Xiaobo Gong[4]*

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ABSTRACT

The blood shows complicated rheological behaviors due to complex fluid-structure interactions of plasma and blood cells. Understanding the rheological features in a finite inertial range in curved pipes is important in designing microfluidic cell-sorting devices. A single capsule behavior in curved pipes has been investigated at finite Reynolds numbers [1]; however, much is unknown how inertial flows with multiple capsules generate both axial and in-plane flow fields. In this study, large-scale simulations are performed for inertial flows of suspension of deformable capsules mimicking red blood cells in toroidal tubes. The immersed boundary method was applied for the fluid-capsule interaction, where the fluid is assumed as an incompressible Newtonian fluid and the capsule membrane is modeled by a hyperelastic material with bending resistance. An in-house code for a fluid-capsule interaction solver [2] was developed, in which a hybrid parallelization with OpenMP and MPI is implemented for both fluid meshes and material points of capsule membrane. We applied various values for the hematocrit (Ht), a volume ratio of capsules to toroidal tube, from 0 to 25%. In our simulations, an axial velocity profile at low Ht is similar to that of a well-known curved pipe flow [3], whereas at high Ht the profile shows a similar trend with a suspension of capsules in straight tubes, where two different velocity regimes arise due to aggregation of capsules in tube center. A snapshot for the in-plane velocity on a tube cross-section shows a non-organized flow field at high Ht, whereas its spatiotemporal average in the axial direction shows a well-organized secondary flow with two counter-rotating vortices, known as Dean vortex. Relative magnitudes of the in-plane velocity to the axial velocity are reduced when increasing Ht. To reveal a mechanism of this reduction, we introduced a macroscopic non-Newtonian model, in which spatial variation of dynamic viscosity is considered that depends on a distribution of local hematocrit obtained by a large-scale simulation. Our investigation predicts two possible mechanisms, which are energy dissipation due to capsule-capsule interactions and macroscopic viscoelasticity of capsule-rich suspension, would reduce the level of secondary flow even though the same level of axial velocity is maintained.

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Deep and machine learning methodology in the context of application to computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREDICTION OF MICROSTRUCTURES OF DENDRITE CRYSTALS AND PROCESS PARAMETERS FOR THERMOPLASTIC RESIN BASED ON MECHANICAL PROPERTIES USING THE CONDITIONAL DIFFUSION MODEL

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ABSTRACT

In this study, we construct a conditional diffusion model that suggests the optimal microstructure and temperature for polyphenylene sulfide (PPS), which commensurate with a desired elastic modulus. PPS is a thermoplastic resin often used in carbon fiber reinforced plastics. During the solidification of thermoplastic resin, the microstructure of dendritic crystal is generated. Typically, the macroscopic mechanical properties are determined from the microstructure. Here, in engineering, these microstructures are affected by the process temperature, which governs the macroscopic mechanical properties. This process temperature is still decided by several expensive experiments. Using the framework of inverse analysis with conditional diffusion model, we aim at predicting the process temperature from the desired macroscopic elastic modulus as inputs. In this way, we can significantly reduce the number of experiments and lead to the effective cycle of PPS manufacturing operations.
The data sets of microstructures of thermoplastic resin are generated by the phase-field method. Nuclei are placed in the initial state as heterogeneous nucleation, and nucleation is considered to probabilistically based on the nucleation rate as homogeneous nucleation. Furthermore, crystal growth from these nuclei is calculated. Then, the extended finite element method (XFEM) is performed on the thermoplastic resin created by the phase-field method to obtain the elastic modulus. We use the elastic modulus as the condition when training the conditional diffusion model. In XFEM, the macroscopic stress is obtained by averaging the stress distribution in each direction by applying three patterns of unit strain, and is used as the value of the elastic modulus. Training data for the conditional diffusion model are the microstructure of the final step in the phase-field method when the crystal has finished growing and the process temperature. The training is performed by adding and removing noise to the set of temperature and microstructure. By adding conditions to the time information during the process of noise removal and addition, the weight of each condition is changed, and it becomes possible to train each condition separately.
Using the conditional diffusion model, we are able to reproduce the detailed microstructure of dendrites. In addition, the model enables us to generate microstructures different from the microstructures of training data. It is shown that a microstructure which satisfies the given conditions is generated and a proper temperature is proposed as a process parameter for the microstructure.

Advances in multi-scale, multi-material, and multi-component Topology Optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FROM VOXELS TO BALLS: TOWARDS CONNECTED PREDICTIONS OF MACHINE LEARNING MODELS IN TOPOLOGY OPTIMIZATION

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ABSTRACT

Although topology optimization has recently seen a multitude of machine learning advances, most algorithms rely on processing and outputting solutions as binary 2D or 3D images. While this state of affairs offers some insight into interpretability and compatibility with existing analysis tools, it suffers from critical drawbacks. Firstly, the massive number of variables, especially in 3D, demand complex and computationally expensive deep learning models. Secondly, the method is highly sensitive to errors, where even minor pixel/voxel inaccuracies can jeopardize structural integrity. Finally, the predicted design solutions often struggle to maintain connectivity, which is essential for load-bearing, and ultimately impact both design performance and manufacturability. These limitations hinder achieving truly optimal structural designs with machine learning models, highlighting the need for alternative approaches.

We explore the use of Maximal Disjoint Ball Decomposition (MDBD) as a new, efficient way to represent and learn shapes in topology optimization as a structured and hierarchical collection of tangent d-dimensional balls and of its associated connectivity graph. Unlike the pixel/voxel approach, MDBD accurately captures optimal designs and enhances their structural connectivity through integration with graph neural networks. Crucially, MDBD requires far fewer parameters, enabling simpler deep learning models, less computational power, and smaller training datasets. At the same time, the connectivity graph of MDBD can be exploited to quantify and enforce the connectivity of the resulting predictions. Therefore, MDBD has the potential to significantly improve the effectiveness and efficiency of machine learning in topology optimization, while maintaining design accuracy and practicality.

Modeling and inverse design of architected materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MINIMUM ACTUATION RECONFIGURATION OF STRAW-LIKE ELEMENTS

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ABSTRACT

Reconfigurable structures having a multitude of carefully designed stable configurations, have a great potential for diverse applications such as deployable and shape morphing structures, as well as architected materials with configuration dependent mechanical properties. Multistability, allowing to stabilize a structure in different configurations can be achieved by embedding it with elements which have instability regions, such as precompressed elastic beams. A promising multistable elastic element discussed here is inspired by the ‘bendy straw’. Under the assumption of planar motion, such straw-like element is modelled as an array of unit-cells having up to four stable equilibria, allowing it to be stabilized in a large number of multiaxial configurations. These elements can be further used to form networks of different geometries and operative stable configurations. For applicability, the transition between different stable configurations of a reconfigurable structure should be done with a minimal number of actuators, which raises a challenge of path finding in a highly nonconvex energy landscape.

Here we focus on minimal actuation reconfiguration of a single straw-like element. For this we begin by setting up the theoretical foundations and introduce a numerical scheme used to describe its mechanical behavior under prescribed relative translational and rotational displacements between its ends. Next, we present an algorithm based on the Nudged elastic band (NEB) method, which is utilized to find the boundary conditions needed to be applied to the straw, for a wanted reconfiguration. These theoretically obtained boundary conditions are then applied to the forward numerical simulation, as well as to an actual straw utilizing an XY-Theta stage, to validate that the wanted reconfiguration is achieved. It should be noted that the presented method can be employed in various multistable systems in order to find the actuation needed to be applied by a set of actuators to cause a wanted reconfiguration, given that the actuation scheme can cause the desired reconfiguration.

Recent advances in computational fracture mechanics and failure analysis
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NOVEL PERIDYNAMICS ELASTIC-PLASTIC FATIGUE DAMAGE MODEL FOR PREDICTING CRACK BEHAVIOR INCORPORATING ELASTO-PLASTIC DEFORMATION FIELD

Dongjun Bang[1] and Ayhan Ince[1]*

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ABSTRACT

Currently, no fatigue damage model has been established that incorporates the nonlocal damage concept by considering the elasto-plastic deformation field. Understanding short crack behavior is complex, and current approaches that focus only on fatigue damage at a single material point instead of within a finite material volume, cannot accurately model abnormal behavior in short cracks [1]. The different mechanisms driving short and long crack propagation require distinct modeling approaches to address the unique nature of damage mechanics in these crack regimes. Hence, a new peridynamics (PD) model has been developed to predict short crack behavior by considering the evolution of elasto-plastic mechanical fields around growing cracks to consider the non-local nature of the damage mechanism. Recently, the authors developed a PD fatigue damage model specifically accounting for R-ratios to simulate crack growth behavior in long cracks within the elastic state [2-3]. Acknowledging the significant influence of local elastic-plastic mechanistic fields on short crack behavior, the authors have expanded the original PD fatigue model to develop a novel PD elastic-plastic fatigue damage model capable of simulating crack propagation in both short and long crack regimes, while incorporating nonlocal damage and elastic-plastic mechanistic fields associated with a propagating crack. Additionally, a new PD elastic-plastic material model is integrated with a PD fatigue damage model. This integration enables simulation not only of crack propagation but also of the actual elasto-plastic stress, strain, and displacement fields around propagating cracks. The elasto-plastic PD fatigue model can simulate damage behaviors across various length scales for crack growth in both short and long crack regimes. To validate the model, predictions of crack growth modes are compared with mechanistic deformation fields for crack growth in various metallic alloys like 2024-T3 and 7075-T6 aluminum alloys. Results demonstrated a close match between model predictions and experimental crack and mechanical deformation data under various R-ratios loading conditions.

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Modeling and inverse design of architected materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MECHANICS OF QUASI-PERIODIC TWO-DIMENSIONAL TRUSS METAMATERIALS

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ABSTRACT

To date, the design of architected materials (or metamaterials) has mostly been limited to periodic configurations, with extensions to gradually varying local periodicity, or irregular architectures that are usually built by adding disorder to primitive periodic architectures. In contrast, quasicrystalline designs (inspired by atomic quasicrystals) are rarely considered. While they do not exhibit translational periodicity, quasiperiodic lattices retain long-range order and exhibit symmetries which are forbidden in periodic materials, such as 5,7, 8 and 10-fold rotational symmetries in the plane. The consideration of quasiperiodic structures leads to a largely unexplored design space for architected materials and consequently to an untapped property space that promises materials with unprecedent features, potentially surpassing the performance of their periodic counterparts in applications relying on lightweight, stiff, and impact-resistant materials.

This talk will describe recent progress on the exploration of the mechanics of two-dimensional quasi-periodic architected materials. A class of two-dimensional truss metamaterials that are inspired by quasicrystal tilings such as the canonical Penrose and Ammann-Beenker tiles is considered. First, the linear stiffness properties of the designs are characterized and compared to classic two-dimensional trusses such as the square, triangular and hexagonal lattices. Among our findings, we show that the quasicrystal designs are isotropic in the linear regime and may exhibit a mixture of bending and stretch-dominated deformation mechanisms. While purely stretch-dominated periodic truss lattices achieve higher linear stiffness, they usually suffer from global buckling instabilities, which significantly hinder their energy absorption capabilities under large nonlinear deformation. Indeed, our simulations confirm that quasicrystal designs avoid global buckling instabilities and only experience localized buckling, leading to designs that may surpass periodic trusses in terms of nonlinear energy absorption. Preliminary experimental results for additively manufactured samples under uniaxial compression are shown to support our findings, and possibilities for future work are also discussed.

A COLLOCATION MODEL REDUCTION SCHEME FOR PDES (CMOR)

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ABSTRACT

Model reduction essentially involves seeking the solution to a partial differential equation (PDE) in a vector space of small dimension compared to the high-fidelity problem. This search is typically performed using the residual of the underlying numerical model associated with the solution of the PDE, either by minimizing it in a suitable norm or by determining the solution in such a way that the residual is orthogonal to an appropriate test space. This operation typically requires a step called hyper-reduction to compute the residuals on a modest number of discretization points. In this presentation, we will demonstrate an approach that departs from this now-classic method and relies solely on the numerical scheme used, or chosen, for the integration of the initial model, while conducting this operation with an extremely reduced number of mesh points. These points are obtained through a numerical quadrature technique. Examples related to finite difference schemes, ADER, and DG schemes will be presented.

Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL INVESTIGATION ON THE STRENGTH OF BI-MATERIAL JOINT FABRICATED BY WIRE ARC ADDITIVE MANUFACTURING

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ABSTRACT

Wire Arc Additive Manufacturing (WAAM) is a prominent Additive Manufacturing (AM) method because of its ability to use different metallic and composite materials. A majority of research efforts on WAAM have focused on singular material fabrication. As multiple combinations of materials can achieve the desired performance more easily than a single material, the investigation of the interaction between different materials can provide guidance for more practical applications. To complement experiments and alleviate research cost and time, numerical models are beneficial. This work aims to model and predict the bond strength of a bi-material joint fabricated by WAAM using the commercial Finite Element Analysis (FEA) software package LS-DYNA. The joint configuration comprises a layer of 17-4 PH alloy and another layer fabricated from Inconel alloy 625. Two typical methods, automatic surface-to-surface contact tie break and cohesive element, are used to study the mechanical behavior between two different materials (i.e., 17-4 PH alloy and Inconel alloy 625) in LS-DYNA. Automatic surface-to-surface contact is extensively used to simulate the interaction between different materials, making it suitable for multi-material joints. Cohesive elements enable the simulation of adhesive joints where materials are bonded together. It provides an accurate representation of the behavior at the bonded interfaces. This allows the fracture prediction in the adhesive bonding of two materials. Specifically, the properties of the interface layer are obtained through experiments on the mechanical characterization of printed multi-material WAAM samples. To validate the effectiveness of the two established simulation methods, the stress-strain curves and fracture obtained by simulation are comprehensively compared with the experimental results via a joint fabricated with 17-4 PH alloy and Inconel alloy 625 in WAAM subjected to the uniaxial tension. The comparison between simulation and experiment demonstrates the fidelity of the numerical models in capturing the intricate complexities of the bonding types. The advantages and disadvantages of using automatic surface-to-surface contact and cohesive elements bonding are comprehensively discussed. Future work will investigate the effects of microstructures on the mechanical behavior of the bi-material joint.

keywords: Wire arc additive manufacturing; Finite element analysis; Bi-material joint; Uniaxial tension

Deep and machine learning methodology in the context of application to computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CNN-BASED SURROGATE MODEL AND TEMPERATURE PREDICTION METHOD USING SUPERPOSITION PRINCIPLE

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ABSTRACT

A CNN-based surrogate model is being developed to speed up CFD calculations.The larger the scale of training data, the higher the cost of training data creation.Therefore, it is difficult to exhaustively learn all shapes, materials, and part arrangements, etc., and improving generalizability is an issue.We referred to the methods of transfer learning and fine tuning, which are often used in the field of image recognition, but it was difficult to create a surrogate model with high generalizability.Therefore, we propose a temperature prediction method using the principle of superposition as one of the solutions to this problem.Among the three forms of heat transfer, i.e., heat conduction, radiation, and convection, the superposition principle holds for heat conduction.By taking advantage of this property, we have devised a method to predict the temperature distribution of multiple heating elements in a circuit board individually, and then fuse these elements to predict the temperature of the entire model.Since the principle of superposition does not hold for radiation and convection, the prediction accuracy is poor if the individually predicted temperatures are only superimposed. Based on the relationship between the temperature after superposition and the temperature difference predicted individually, we corrected the temperature after superposition to improve the accuracy.

Phase-field modeling: Analytics, benchmarks, and discussions
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA ASSIMILATION USING IN SITU OBSERVATION DATA FOR HIGH-FIDELITY PHASE-FIELD SIMULATION OF SOLID-STATE SINTERING

Akimitsu Ishii[*1], Akinori Yamanaka[2], Mizumo Yoshinaga[3], Shunsuke Sato[3], Ikeuchi Midori[3], Satoshi Hata[3], Hikaru Saito[3] and Akiyasu Yamamoto[2]*

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ABSTRACT

Sintering is a fundamental technology for manufacturing various materials. To improve the mechanical, electrical, magnetic, and other properties of sintered materials, it is necessary to understand, predict, and control the microstructural evolutions and structure formulation during sintering. Cutting-edge experimental techniques have realized the four-dimensional (three-dimensional space and time) observation of microstructural evolution during solid-state sintering [1]. Although such experiments provide various useful information, the sintering behavior has not been fully observed due to some limitations in target materials, experimental equipment, and experimental conditions.

Phase-field (PF) method is a powerful numerical methodology for solving free-boundary problems occurring at nano- and mesoscales, and thus it has been used in several recent studies to understand the microstructural evolution during solid-state sintering [2]. Because the PF model is a continuum one, accurate material parameters such as physical values and model parameters are required to perform PF simulation quantitatively. However, many material parameters of sintered materials are largely unknown and some of them are difficult to identify experimentally.
Recently, data assimilation (DA) has attracted attention as an effective method for the inverse estimation of unknown material parameters from small experimental datasets. DA integrates time-series experimental data and numerical simulation results based on Bayesian inference. In the previous study [3], a DA method using tree-structured Parzen estimator (DMC-TPE) is applied to a PF simulation of solid-state sintering, and it is demonstrated through a numerical experiment that DMC-TPE can estimate multiple temperature-dependent material parameters with high accuracy. However, no study has reported the estimation result from DA using actual experimental observation data of solid-state sintering.

In this work, we achieved to perform high-fidelity PF simulation of solid-state sintering with copper nanoparticles by estimating the material parameters via DMC-TPE using morphological data observed using an in situ scanning transmission electron microscopy and PF simulation results. The high-fidelity PF simulation quantitatively predicted the sintering behavior.
This work was supported by JST CREST (JPMJCR18J4).

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Recent advances in meshfree and particle methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATION OF PARTICLE METHOD TO MIXING PROCESS SIMULATION

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ABSTRACT

There is a high demand for efficient mixing of multiple liquids in small quantities in the manufacturing process of industrial products. For example, when stirring two liquids in a small amount in a vessel, in addition to mixing the two liquids, it is necessary to simulate the three-phase multi-phase flow, including bubbles that are entered due to the waves of the liquid surface generated during mixing. Under conditions where the amount of liquid is small, it is also necessary to consider the effect of the surface tension generated on the liquid surface. Simulations using conventional computational mesh are effective in predicting the flow of the liquids in the vessel as well as predicting the waves of the liquid surface. However, high-resolution computational mesh is required to predict the mixing process considering the interaction between the two liquids and bubbles. In simulating such the mixing processes, the particle method is an effective approach. The simulation using the particle method (moving-particle semi-implicit method [1]) has an advantage that can reduce the deterioration of prediction accuracy affected by the resolution of the computational mesh shown above. For these reasons, we investigated the application of the mesh and the particle methods to the simulation of the mixing process of multi-phase flow consisting of two liquids and bubbles. By using the mesh method, it was possible to predict the flow of the liquid in the vessel and the waves generated on the liquid surface with a small calculation time. Furthermore, by using the particle method to predict the mixing process phenomenon caused by the interaction between two liquids and bubbles, highly accurate prediction was possible. The simulated results were verified using experimental results. The liquid surface shape generated on the liquid surface of the liquids was in good agreement with the results of the experiment. In addition, it was clarified that the mixing phenomenon caused by the interaction of two liquids and bubbles can qualitatively reproduce the phenomenon shown in the experiment.

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Multi-scale, multi-rate damage and fracture: Models, experiments, and simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INVESTIGATION OF A NOVEL LASER-INDUCED SPALLATION METHOD: ANALYSIS OF SHOCK AND SPALL BEHAVIOR THROUGH ATOMISTIC, FINITE ELEMENT, AND THEORETICAL MODELING

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ABSTRACT

In this talk, we discuss a novel laser method for studying material spall behaviour. Here, the front and back surfaces are irradiated with a laser, resulting in the formation of two pressure pulses that contain a leading compressive wave and an unloading tensile wave. When the superimposition of these two unloading tensile waves produces a state of hydrostatic pressure that exceeds the spall strength of the material, failure occurs. To investigate this method, perfect Nickel crystals were photo-excited using femtosecond laser pulses in atomistic simulations, and the laser-metal interactions were simulated using a two-temperature master equation. Our results show that the two-pulse laser configuration can induce spallation in the material, and the resulting spall strength can be traced through the material's free surface velocity. The mechanism of spallation, i.e. void nucleation, growth, and coalescence, was observed, and it is seen that the formation of stacking faults and Shockley partials is critical. In addition, failure of an imperfect Nickel crystal revealed that the presence of a pre-existing void increases dislocation emission when compared to a perfect crystal. Next, it was shown that the type of laser-induced damage can be controlled by tuning the laser fluence, pulse duration, and initial temperature. Finally, a macro-scale FEM model was developed to reproduce spall behaviour, and it was that by delaying one of the pulses, the location of spall plane can be controlled.

Complex fluid flows in engineering: Modeling, simulation, and optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A COMPUTATIONAL FLUID DYNAMICS APPROACH FOR METAL HYDRIDE HYDROGEN STORAGE

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ABSTRACT

Metal hydride hydrogen storage (MHSS) systems offer promising solutions for efficient and safe hydrogen storage. However, the low thermal conductivity of metal hydride materials poses challenges to hydrogen absorption kinetics. Therefore, this study aims to address this issue by applying a passive technique of various heat exchanger designs and enhancing the thermal performance of the MHSS system. This study investigates the performance of MHSS systems employing different heat exchanger configurations, including internal and external heat exchangers, to improve hydrogen absorption kinetics. The combination of internal semi-cylindrical coil heat exchangers (SCHE) with external heat exchangers such as phase change materials (PCM) and cooling jackets (CJ) is examined. The study evaluates hydrogen absorption kinetics, average bed temperatures, and reaction fractions across different MHSS designs through simulations and analyses. The methodologies involve computational modelling based on energy equations governing the hydrogen absorption process and thermo-physical properties of metal hydride alloys and PCM. Results demonstrate that integrating internal and external heat exchangers significantly enhances hydrogen kinetic reactions, leading to faster absorption rates. Incorporating PCM and cooling jackets facilitates rapid temperature reduction during absorption, consequently improving hydrogen reaction fractions. Compared to the standalone SCHE configuration, the combination of SCHE with PCM and CJ reduces absorption duration by 37.72% and 50.69%, respectively. This study highlights the potential of combined heat exchanger systems to enhance MHSS performance and offers insights into optimising hydrogen storage technologies for industrial applications. The findings underscore the importance of efficient heat transfer mechanisms in accelerating hydrogen absorption kinetics. Moreover, the study highlights the significance of integrating internal and external heat exchangers to optimise MHSS designs for improved energy storage and utilisation. In future applications, the insights gained from this study could inform the development of advanced MHSS systems with enhanced hydrogen absorption capabilities. Further research may explore the optimisation of heat exchanger configurations and investigate the scalability and practical feasibility of implementing optimised MHSS designs in industrial settings.

Data-driven methods for modeling complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODEL REDUCTION OF THE PLASMA KINETIC EQUATIONS

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ABSTRACT

We propose a data-driven projection-based reduced-order model (ROM) to reduce the computational cost of the spectral plasma solver (SPS) of the Vlasov-Poisson equations. The SPS solver is based on a Fourier spectral expansion in space, asymmetrically-weighted Hermite expansion in velocity, and an implicit temporal integrator. The main advantages of the SPS solver are its conservation and fluid-kinetic coupling properties, where the first three expansion coefficients correspond to the macroscopic description of the plasma, while higher-order expansion coefficients correspond to higher-order fluid moments capturing the kinetic effects of the plasma. A core contribution of this work is to introduce a reduced-order model for the kinetic effects into SPS while keeping the macroscopic description intact. We show that this preserves its fluid-kinetic property, and conserves mass, momentum, and energy. Moreover, the suggested strategy overcomes the nonlinear bottleneck by efficiently handling convolutions. The numerical results show that our method can adequately emulate the SPS simulations at a fraction of the cost, which we test on the following benchmark problems: 1D-1V weak Landau damping, 1D-1V bump-on-tail instability, and 2D-2V current-driven ion acoustic instability.

Large-scale structural and fluidic topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CFD-MRI: CHARACTERIZATION OF REACTIVE FLOWS BY SOLVING INVERSE PROBLEMS

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ABSTRACT

Catalytic processes are of tremendous importance: many everyday life products and technologies require catalysts. Improving heterogeneous catalytic processes in a chemical reactor often necessitates detailed knowledge of concentration, velocity, and temperature distributions. Magnetic resonance imaging (MRI) can measure those distributions noninvasive and spatially resolved, presenting a clear advantage compared to conventional techniques as they are often invasive and only capable of measuring locally. In our project, we develop a combined framework of computational fluid dynamics (CFD) and MRI wherein we solve two inverse problems to characterize heterogeneous reactive flows. In the first step, we utilize an adjoint-based topology optimization approach to obtain the porous structure from the measured velocity distributions. The flow field is computed by solving the discrete porous media BGK-Boltzmann equation, which approximates the homogenized Navier-Stokes equations in the hydrodynamic limit. In the second step, we identify reaction rate parameters from given concentration distributions using algorithmic differentiation and a lattice-Boltzmann method (LBM) to approximate the system of reaction-advection-diffusion equations. In both steps, we solve the conservation equations as side constraints of our optimization problem, ensuring the physical behavior of the flow and concentration fields. As MRI measurements suffer from a relatively low signal-to-noise ratio (SNR), we aim to reduce the ”non-physical” statistical noise from the velocity and concentration distributions via the presenting method.

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Constitutive modeling of complex materials with machine learning and artificial intelligence
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING OF SOFTENING PHENOMENA IN ELASTOMERS BY DEEP SYMBOLIC REGRESSION

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ABSTRACT

Rubber-like materials exhibit pronounced softening after the very first loading cycle. This phenomenon, known as the Mullins effect, plays an important role in the stress-strain response not only of elastomers but also soft biological tissues. Despite numerous modeling approaches proposed in the last years in literature, accurate prediction of the Mullins effect, especially under complex loading conditions, still remains a challenging task.

In this contribution, we propose a novel method to model the Mullins effect using deep symbolic regression [1]. The first goal is to find an algebraic expression of a strain energy which fits the given experimental data from the primary loading as accurately as possible. By incorporating the continuum mechanical framework, the method combines the advantages of known physical relationships with the unbiased optimization approach of symbolic regression. The procedure has already been applied to discover incompressible hyperelastic material models and is benchmarked against the generalized Mooney-Rivlin model [2]. In the second step, the method is extended to inelastic effects. To this end, stress-strain data of unloading and secondary loading are artificially created by the Ogden-Roxburgh model [3] and described again by the deep symbolic regression. In addition, the proposed model is tested on an experimental temperature-dependent data set. Good agreement between the so obtained material models and the experimental data is demonstrated.

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Deep and machine learning methodology in the context of application to computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INVESTIGATION OF CNN-BASED MULTIGRID-BIDIRECTIONAL NETWORKS

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ABSTRACT

A technology to super-speed physics simulation by deep learning is under development. This ultra-fast technology can speed up calculation speed by a factor of several hundred to a thousand, which is expected to improve design efficiency and performance quality through optimization. Significant reductions in design time can be realized by allowing design changes and performance and quality evaluations to be performed interactively. In design optimization, it is necessary to run physical simulations under a very large number of conditions, and in the past, the design parameter space to be explored was sometimes limited. However, by greatly speeding up the physical simulation, it becomes easier to search in a wide parameter space, and optimal solutions with fewer omissions can be obtained.

Currently, we are developing a multi-grid CNN-based network for models with a mixture of coarse and fine grids (dense grids) as a technology to address the issues of model scaling (high-definition), insufficient hardware specifications, and increased training man-hours. We are working on the development of a multi-grid CNN-based network for models with mixed coarse and fine grids.

As a basic study, a technique for propagating physical information from one coarse grid to one dense grid has already been reported at a conference on Computational Engineering and Science (June 2023: Application of CNN-based multi-grid networks to CFD). This time, we developed a technique that enables bidirectional propagation of physical information between the coarse and dense grids, as well as prediction with three basic networks without limiting the number of grids, and applied it to a basic temperature distribution prediction model for circuit boards. This report describes the results of applying the technology to a basic temperature distribution prediction model for circuit boards.

This technology is not limited to temperature prediction, but can be widely applied to simulations that predict the spatial distribution of physical quantities.

Lattice Boltzmann modelling and study of complex flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LATTICE BOLTZMANN SIMULATION OF POLLUTANT DISPERSION USING EULERIAN AEROSOLS MODELS: APPLICATION TO NATURAL VENTILATION INSIDE BUILDINGS

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ABSTRACT

Lattice Boltzmann method (LBM) has been used successfully in the field of urban flow simulation such as pollutant dispersion in recent years [1] thanks to its interesting numerical properties (low numerical dissipation, easy implementation for parallel simulation). However, it has mainly been used for pollutant dispersion in urban areas (outside flow) recently rather than for simulation of air quality and natural ventilation inside buildings.
This study presents the extension of previous work [1] based on the hybrid recursive regularized lattice Boltzmann model (HRR LBM [2]) to the simulation of natural ventilation inside buildings. Gaseous transport equation method previously used in different studies are compared with an aerosol model in Eulerian framework implemented in the lattice Boltzmann solver. The different LB simulations are validated with experimental [3] and numerical [4] data on a configuration of pollutant release inside a building with open windows immersed in an atmospheric boundary layer. The accuracy of obtained results is evaluated using the quality criteria introduced in Chang and Hanna [5] in order to evaluate the performance of the proposed LB model for air quality studies.
Depending on the data available in the literature, the accuracy and computational cost of the proposed method will be compared to Eulerian and Lagrangian aerosol model in the Navier Stokes framework to evaluate the interest of using LBM for such applications.

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Constitutive modeling of complex materials with machine learning and artificial intelligence
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ON AUTOMATED DISCOVERY OF THERMODYNAMICALLY CONSISTENT FINITE STRAIN PLASTICITY MODELS

Asghar Arshad Jadoon[*1], Knut Andreas Meyer[2] and Jan Fuhg[1]*

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ABSTRACT

Constitutive modeling lies at the core of mechanics, allowing us to map strains onto stresses for a material in a given mechanical setting. Historically, researchers relied on phenomenological modeling where simple mathematical relationships were derived through experimentation and curve fitting. After the recent revival of machine learning, the community started exploring the idea of modeling constitutive behavior through neural networks. It started with a purely data-driven, black-box approach where the neural network could assume any arbitrary mapping function as long as it could accurately relate stresses and strains. However, these architectures violated established mechanical principles. Therefore recent efforts concentrate on designing neural network architectures that could incorporate physics and mechanistic assumptions into machine-learning-based constitutive models. For history-dependent materials, these models have so far predominantly restricted to small-strain formulations[1,2].

In this work, we develop a finite strain plasticity formulation based on thermodynamic potentials[3] to model mixed isotropic and kinematic hardening. The goal of this work is an automated discovery framework of hardening models using neural networks that a priori satisfy all thermodynamic constraints. We test our model on experimental uniaxial cyclic-loading data. We show that the framework is able to not only interpolate well but also to extrapolate remarkably to unseen data. This ability to generalize beyond the training set underscores the robustness and predictive power of our model. By automating the discovery of hardening models, our approach eliminates user bias and ensures that the resulting constitutive model complies with thermodynamic principles, thus offering a more systematic and physics-informed framework.

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OPTIMIZATION OF STRUCTURAL INSTRUMENTATION FOR BRIDGE HEALTH MONITORING

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ABSTRACT

The bridge structures are of utmost importance due to their critical role in the transportation network. Data-driven approaches offer promising tools for continuous long-term condition monitoring of such large-scale structures. In this study, time-series segmentation has been utilized for damage detection in a real-case bridge structure. Signals taken from accelerometers installed on the bridge structure are processed to detect damage(s). Instrumentation of the entire bridge structure, however, may be laborious, expensive, and time-consuming. Therefore, the quantity and location of sensors are optimized to yield the most efficient arrangement. The presented approach can contribute to the development of more cost-effective methods for bridge health monitoring.

Data-driven approaches for solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HETEROGENEOUS PERIDYNAMIC NEURAL OPERATORS (PNO): TOWARDS CONSTITUTIVE LAW AND MICROSTRUCTURE DISCOVERY

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ABSTRACT

In this work we introduce the heterogeneous peridynamic neural operator (PNO) approach, for data-driven constitutive modeling of heterogeneous materials. The goal is to learn both a nonlocal constitutive law together with the material microstructure from loading field-displacement field measurements. To this end, we propose a two-phase learning approach. First, we learn a homogeneous constitutive law in the form of a neural network-based kernel function and a nonlocal bond force, to capture complex homogeneous material responses from data. Then, in the second phase we fix the learnt bond force and fine-tune the kernel function for each material point, so as to capture the material heterogeneity. Owing to the state-based peridynamic skeleton, our PNO-learned material models are objective and have the balance of linear and angular momentum guaranteed. In this study, the new PNO architecture learns a constitutive model for a biological tissue with anisotropic heterogeneous response undergoing large deformation regime. The anisotropy and heterogeneity of this tissue stems from collogen fibers with unknown natural orientation, resulting in a location-dependent anisotropy. To demonstrate the applicability of our approach, we apply the heterogeneous PNO in learning the material model and fiber orientation field from digital image correction (DIC) data containing the planar displacement field on the tissue in a biaxial test. The learned orientation angles are validated against experimentally detected fibers.

Mechanobiology of cells, vesicles and biomembranes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MODIFIED HELFRICH MODEL FOR LIPID BILAYERS

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ABSTRACT

The curvature of the biological membrane is a crucial aspect of many cellular processes like tubular formations, invaginations, fusion, and budding [1]. The Helfrich model is a widely used continuum model that describes the bending energy of cellular membranes as a function of their curvatures - mean and Gaussian.

In this work, we present a modified Helfrich model aimed at providing improved control over the asymmetric morphological changes in biological membranes. We conduct a comparison of the stresses and moments generated by our model with those of the classical Helfrich model and another modified Helfrich model introduced in [2].

The membrane surface and its large bending deformations are modeled as a liquid shell using curvilinear coordinates. The finite element approach to solve the resulting equation requires C1-continuous discretization for which NURBS-based isogeometric finite elements are used. Furthermore, we analyze a numerical example related to the budding process, similar to the work in [3].

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Methods for identification, machine learning, and uncertainty quantification of reduced order models of coupled systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NONINTRUSIVE COMPUTATION OF INVARIANT MANIFOLDS AND THEIR REDUCED DYNAMICS IN LARGE NONLINEAR FINITE ELEMENT MODELS

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ABSTRACT

Invariant manifolds, in general, and Spectral Submanifolds (SSM), in particular, have emerged as rigorous and predictive model reduction tools for nonlinear dynamical systems. Recent developments have enabled direct computation of invariant manifolds and their reduced dynamics for high-dimensional finite-element (FE) models by solving the associated invariance equations in physical coordinates using only the eigenvectors associated with the master modal subspace. However, FE models in commercial solvers generally do not provide information on the nonlinearities required for the direct approximation of invariant manifolds.

In this talk, we show how to overcome this limitation using a nonintrusive construction of invariant manifolds and their reduced dynamics in both equation-driven and data-driven environments. Specifically, in the data-assisted setting, we use a small number of unforced FE simulations to learn SSM-based ROMs and use these ROMs to predict the forced response of the FE model without performing any costly forced simulation. We demonstrate our methods a range of nonlinear mechanical systems from simple structures, such as beams and shells, to more complex geometries, such as a micro-resonator model containing more than a million degrees of freedom.

Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SENSITIZING THE RANS APPROACH TO A SCALE-RESOLVING COMPUTATIONAL FRAMEWORK FOR COMPLEX MULTI-PHYSICS TURBULENT FLOWS

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ABSTRACT

The present work deals with the scale-resolving simulation of complex multi-physics turbulent flows. The complexity of flow refers to a variety of differently structured flow and heat-transfer phenomena including plasma-actuated flow control relevant to aircraft and car aerodynamics, internal-combustion engines and corresponding cooling channels, two-phase flow in bubble columns, particle dynamics in pipes, physiological flows in the human aorta, flows around blunt bodies, thermal mixing in cross-stream type T-junctions, flow in a concentric annulus subjected to inner/outer cylinder rotation and complex duct and pipe configurations characteristic of various industrial applications. Comparative evaluation of the results with reference databases from relevant experimental and numerical studies shows the correctly predicted instantaneous character of the flow as well as its averaged pattern [1-3]. The anisotropic turbulence residing in unresolved motion is described by a RANS-based (Reynolds-averaged Navier-Stokes) eddy-resolving closure that accounts for the dynamics of the entire subscale stress tensor. The eddy-resolving capability of the model is enabled by the introduction of an additional production term into the length-scale determining equation. Its functional dependence is motivated by the Scale-adaptive Simulation (SAS) strategy by Menter and Egorov (2010, FTaC 85:113-138). The essence of this term is its dependence on the second derivative of the underlying velocity field, providing the rationale for its definition originally introduced by Rotta (1972), which adequately implies the recognition of the inhomogeneity of the flow that occurs specifically in the shear layer regions, with an emphasized inflection of the velocity profile, and promotes the detection of flow structures. This RANS-based Reynolds-stress model, sensitized to the turbulent fluctuations, brings important advantages. This primarily concerns the grid spacing-independent model formulation, which is particularly effective for arbitrarily complex grid cell arrangements.

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Modeling and simulation of advanced manufacturing processes for metals
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ATOMISTIC SIMULATION OF COLD SPRAY PROCESS FOR ALCOCRFENI HIGH-ENTROPY ALLOY

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[1]*University of Alberta*

ABSTRACT

Cold spray deposition is a widely used solid-state surface coating technology. In this process, micron-scale solid particles are deposited on a substrate at high velocities causing severe plastic deformation, thus resulting in buildup of a coating. In contrast to thermal spray deposition, the particle temperature in the cold spray process remains below the melting point of the feedstock material. This helps prevent oxidation and phase changes during the process, making it ideal for various engineering applications. Despite several experimental studies on cold spray deposition, understanding the bonding phenomenon involved is difficult due to the complex mechanisms that occur at the nanometer scale. Recent simulations suggest that the bonding mechanism may involve a combination of impact-induced jetting, formation of adiabatic shear bands, and hydrodynamic spall.

The present study explores these phenomena using molecular dynamics simulations. A series of atomistic simulations were conducted for AlCoCrFeNi high-entropy alloy particle impacting an Fe substrate, considering variations in particle size and velocities. Interfacial jetting is observed at high impact velocities. Based on the simulation results, the optimal parameters for achieving a dense and uniform coating of the high-entropy alloy on the substrate are also identified. The coating performance is quantified using the horizontal and vertical flattening ratio of the particle. The results obtained can be instrumental in the design and parameter optimization of the cold spray process for high-entropy alloy deposition.

Keywords: Bonding Mechanism, Cold Spray Deposition, High-entropy Alloy, Molecular Dynamics Simulation, Parameter Optimization

Emerging topology and shape optimization techniques in computational design of materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION OF GEOMETRICALLY NONLINEAR COMPLIANT MECHANISMS WITH VARIABLE LOADS AND SUPPORTS

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ABSTRACT

In this study, we present a novel method for performing design synthesis of compliant mechanisms in which the locations of the fixed supports and applied loads are subject to optimization along with the internal material distribution. Previous studies have demonstrated that by including the load and support locations as design variables, one can achieve significantly enhanced performance when compared with designs whose loads and support locations are selected arbitrarily or by intuition [1]. The current work extends this method to a variety of more complex design problems. In the examples presented, the compliant mechanisms all exhibit large, geometrically nonlinear displacements. To solve the nonlinear elasticity problem, we implement a modified nonlinear Neo-Hookean hyperlelastic model and we compute the displacements using nonlinear finite element analysis. The equilibrium equation is solved using a displacement-control method, and we compute sensitivities using a discrete adjoint formulation. In order to prevent large mesh distortion in regions where the material density is low, we continuously interpolate between the nonlinear elasticity model, and a linear elasticity model, which is applied only in low-density regions.

In earlier work, we developed an original super-Gaussian projection method for parameterizing the support locations [1]. Here we extend this method to accommodate both variable support locations and input displacement orientation as design variables. We demonstrate our method by performing topology optimization of three example mechanisms: a gripper with maximum displacement at the jaws, an airfoil with snap-through displacement for actuation of the trailing edge, and an airfoil with path-following displacement at the leading edge. In each example, the optimized mechanism outperforms an analogous design in which the support locations and load orientation are fixed during the optimization.

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Imaging and computational methods for biomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A FREE SOFTWARE APPLICATION FOR ONE-CLICK STRESS COMPUTATION OF ABDOMINAL AORTIC ANEURISM

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ABSTRACT

Abdominal aortic aneurysm (AAA) refers to a permanent and irreversible dilation of the lower aorta. Symptomless, AAA can expand to the point of rupture if left untreated. Based on mechanics, an artery ruptures when the local wall stress exceeds the local wall strength. Therefore, the AAA wall stress, determined reliably and quickly through non-invasive approaches, can help with patient-specific treatment. BioPARR (Biomechanics based Prediction of Aneurysm Rupture Risk) is a free software package for AAA stress analysis based on finite element (FE) method [1]. Fed with the patient's blood pressure and the AAA and intraluminal thrombus (ILT) label maps extracted from the medical images, BioPARR conducts automatic robust computations based on the contemporary computational biomechanics approaches that obviate the requirement for patient-specific material properties [2]. As a truly patient-specific approach based solely on the clinical data, BioPARR presents a clinically applicable standardized approach for comparative evaluation of AAA.

While seamless at the time of release, BioPARR can be improved based on recent software advancements. BioPARR relies on multiple libraries and external software, e.g., 3D Slicer image computing platform, ParaView, and Abaqus. It functions optimally with the recommended versions of these external software, but subsequent updates may compromise BioPARR's robustness. Generally, the recommended older version of freeware may lack adequate support for new hardware and operating systems. Hence, BioPARR requires updates and maintenance, aligned with updates to the external software. Another limitation involves using expensive software like Abaqus, though it could potentially be substituted with freely available FE packages.

In this presentation, we introduce a one-click free software application for AAA stress analysis developed based on MATLAB programming language. The redistributable application is a royalty-free standalone single executable file that is automatically installed on a typical system with no specific hardware requirements. During installation, it automatically fetches and installs MATLAB Runtime as a collection of shared libraries, MATLAB code, and other files that enable the execution of compiled and packaged MATLAB applications on systems without an installed version of MATLAB. The frontend provides a user-friendly window for the end user to input the required data. A single click on the application window initiates the backend computations and visualizes the AAA stress results. The backend utilizes recent MATLAB capabilities, including the Partial Differential Equation Toolbox for FE computations.

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Emerging frontiers and methods in digital manufacturing: Modeling, simulation, and beyond
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPRESSION MOLDING-STRUCTURAL COUPLED ANALYSIS OF SHORT-FIBER REINFORCED COMPOSITE UNDER VARIOUS COMPRESSION MOLDING CONDITIONS

Da-Young Jang[1], Geung-Hyeon Lee[1] and Jang-Woo Han[1]*

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ABSTRACT

Composite structures are typically manufactured through various molding processes such as injection molding, compression molding, resin transfer molding, and so on. These molded structures made by composite materials are widely used in various engineering applications due to its high-stiffness-to-weight ratio and multi-functional properties. Although the many advantages of the Compression molding, a phenomenon must be taken into consideration during the design and manufacturing process is that various flow characteristics can be appeared by the initial conditions of the molding process. Especially in the case of short fiber reinforced composite materials, arbitrary fiber orientation characteristics can be occurred by various flow as well as matrix-fiber interaction characteristics, and these local fiber orientation characteristics can directly impact the mechanical behavior of the molded product.[1]

Therefore, this study investigated the flow and its corresponding local fiber orientation characteristics of short fiber-reinforced composite materials under various molding conditions and conducted molding-structural coupling analysis considering local fiber orientation characteristics in order to provide reliable results during the design process. In addition, the study tried to enhance the accuracy of the molding-structural coupling analysis by considering the matrix-fiber interaction as well as residual stresses.

Compression molding analysis of short fiber-reinforced composite materials under various molding conditions was conducted by using the Moldex 3D software, where the local fiber orientation characteristics depending on the resin flow, matrix-fiber interaction as well as residual stresses were investigated for the various molding conditions. Furthermore, compression molding-structural coupled analysis for the short fiber-reinforced composite materials was conducted by connecting the Modlex3D, Digimat and commercial FE softwares (Ansys and Abaqus). Mean-field homogenization is employed in order to evaluate the effective local anisotropic mechanical properties depending on the fiber orientation, and these local anisotropic properties are mapped in the structural finite element model.

In the numerical study, the mechanical behavior of the ASTM D638 tensile specimens which are manufactured by various molding conditions are investigated to verify the effect of fiber orientation on the local behavior of the short fiber reinforced composite structure.

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Modeling and simulation of the electro-chemo-thermo-mechanical interactions in energy transition and energy storage systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE COMPUTATIONAL MODELING OF ELECTRO-CHEMO-MECHANICAL INTERACTIONS IN STRUCTURAL BATTERY COMPOSITES

Ralf Jänicke[1], David Rollin[1], Vinh Tu[2], Fredrik Larsson[2] and Kenneth Runesson[2]*

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ABSTRACT

The Structural Battery represents an innovative carbon fiber-reinforced polymer composite, designed to serve a dual purpose: As a storage device for electrical energy (viz. as a battery) and as a robust support for mechanical loads. Carbon fibers play a multifaceted role, acting as an active electrode material, current collector, and mechanical reinforcement. These fibers are integrated into a Structural Battery Electrolyte, comprising a solid phase (a porous polymer network) and a liquid electrolyte that facilitates the movement of ions, particularly Li-ions. The ion-mobility is brought about by stress-assisted diffusion (driven by the chemical potential gradient), migration (induced by the electric field), and convection (resulting from fluid motion, i.e., seepage) [1]. In summary, the liquid phase within the porous polymer network promotes ion transport between electrodes, while the solid phase effectively distributes mechanical stresses.

This presentation showcases the capabilities of a recently developed computational two-scale modeling framework, exemplified by [2,3], in evaluating the integrated electro-chemo-mechanical properties of Structural Battery electrode materials. The governing equations of the problem are established upon coupling Gauss law for electric fields and mass conservation for each mobile species with mechanical (quasi-static) equilibrium. By utilizing Variationally Consistent Homogenization, we are able to establish a two-scale model where both the macro- and the sub-scale equation systems emerge from a single-scale formulation. We explore various couplings and their properties across the scales through numerical assessment of the intricate characteristics of Structural Battery composites.

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Mathematics and algorithms for predictive digital twins (DT)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NEURAL PARTIAL DIFFERENTIAL EQUATION MODELS OF COMPLEX DYNAMICAL SYSTEMS

Sanket Jantre[*1], Anthony DeGennaro[1] and Nathan M. Urban[1]*

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ABSTRACT

In science and engineering domains, we often turn to mechanistic computer simulation models to predict the behavior of natural systems, such as fluid dynamics, molecular dynamics, or particle interactions in a collider. These simulations are often based on differential equations and provide critical information about the underlying governing equations but often are computationally expensive. To address this limitation, we explore the use of machine learning based approach, neural partial differential equation (NPDE), which seeks to emulate a complex computer model with a simpler partial differential equation (PDE) whose governing equation or “right hand side” is learned from data in the form of a neural network. As a test case we look at Cahn Hilliard equations for phase separation in self-assembling nanomaterials. We emulate the fast transient behavior in the PDE and incorporate the emulator in solver for time stepping in the extrapolation domain. Subsequently, we will explore ways to quantify the neural network uncertainty via a Bayesian deep learning framework. To recover useful physical equations from limited simulation data, we will also explore the reduction of overparameterized neural network weight spaces through linear subspace methods and Bayesian inference on this reduced parameter space.

Mathematical modeling and simulation for social, environmental, and disaster prevention issues
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTATIONAL APPROACH FOR HYDROGEN COMBUSTION MODELLING OF GRAIN DRYING MACHINE

Sams Jarin[*1], Zhongzheng Wang[1], Md Imran Hossen Khan[2], Nawshad Haque[3] and Emilie Sauret[1]*

[1]Queensland University of Technology
[2]Agridry Dryers Pty Ltd.
[3]CSIRO

ABSTRACT

The drying process is a critical step in agricultural grain processing, contributing significantly to the final product's quality and shelf life. Various drying techniques are employed in the agricultural industry, ranging from traditional methods to more advanced technologies like mechanical and thermal drying. The drying industry heavily relies on thermal drying methods which is highly energy-intensive and contributes to greenhouse gas emissions, worsening the global warming issue. Replacing fossil fuels with green hydrogen fuel in the grain drying process can significantly reduce the greenhouse gas emissions and offer a carbon-neutral solution for powering drying operations. However, the widespread adoption of hydrogen as a fuel faces several challenges, particularly in understanding the complex combustion kinetics of hydrogen fuel. The unique properties of hydrogen, such as its high diffusivity and wide flammability range, pose challenges for effective combustion and mixing dynamics in drying process. Furthermore, there is an urgent demand to develop the advanced mathematical model for simulating the hydrogen combustion processes more accurately for optimizing drying performance. To meet these challenges and develop efficient and clean hydrogen derived drying system, a comprehensive understanding of the mixing and combustion dynamics of hydrogen-oxygen components is essential. This necessitates the use of sophisticated mathematical modelling tools such as CFD model to simulate and analyze the intricate gas dynamics involved in hydrogen combustion. The principal aim of this work is to generate and evaluate an efficient CFD model for the hydrogen combustion process using premixed hydrogen gas for the grain drying process. To simulate the combustion of hydrogen – air, a transient CFD model of energy, turbulence, radiation, and species transport are going to be implemented in the ANSYS Fluent software. This model provides the optimum velocity of hydrogen gas for maximum achievable temperature for a premixed hydrogen combustion CFD model of grain drying operation. To achieve the maximum accuracy from the model, different ratios of hydrogen – air combination are going to be investigated which can then eventually lead to generate a successful new hydrogen derived grain dryers' machine.

Recent advances in high-order methods for computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A FINITE ELEMENT FRAMEWORK WITH GLOBAL DIVERGENCE-FREE CONSTRAINTS FOR NON-STATIONARY NON-LINEAR NAVIER-STOKES EQUATIONS

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ABSTRACT

The Navier-Stokes (N-S) equations characterize the dynamics of fluid flow, capturing phenomena ranging from laminar to turbulent behaviors over time [1,2]. While the N-S equations inherently constitute a non-stationary and nonlinear problem, simplified linear equations are applicable under specific conditions, such as low Reynolds numbers and laminar fluid flow. This project focuses on incompressible fluids, introducing a mathematical model that enforces the divergence-free velocity constraint. Traditionally, the Sobolev space serves as the foundation for determining solutions to the velocity and pressure fields through weak problem formulations. However, this project proposes an alternative approach, decomposing the problem into two distinct subproblems for velocity and pressure. The decomposition is achieved by constructing a divergence-free Sobolev subspace for velocity and its test functions. This innovative approach allows the formulation of a symmetric problem solely for velocity, while the pressure problem is derived by applying the complement of the divergence-free Sobolev subspace for test functions.
In the finite space, an approximation field of arbitrarily high orders is constructed using the standard finite element method. The null-space method [3] is then employed to build a global divergence-free approximation subfield, ensuring compliance with Dirichlet boundary conditions. Subsequently, the approximate velocity field can be calculated using a linear or non-linear approach, depending on the type of N-S problem. The complement of the divergence-free approximation subfield is also constructed using the null-space formulation, facilitating the determination of the approximate pressure field. The effectiveness of this method is demonstrated through representative 2D and 3D examples, encompassing domains with both straight and curved boundaries. The scenarios include linear and non-linear problem formulations, as well as stationary and non-stationary fluid flows. This advantage is particularly pronounced in non-linear formulations, where the iteration procedure focuses solely on the velocity field, with pressure obtained once the velocity is established.

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Buckling analysis and design of thin-walled structures based on novel and intelligent computational methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LARGE DEFORMATIONS OF GRADIENT ELASTIC SHELLS

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ABSTRACT

Based on a generalization of Budiansky's nonlinear shell theory, a novel mechanical formulation for the fully nonlinear gradient shell theory in the large deformation regime is developed. The field equations are obtained in their weak forms based on kinematically exact models. An extension of a linear constitutive equation is presented to capture the effect of an internal material length scale in the shell deformation. An appropriate finite element is developed and used to incorporate the additional degrees of freedom arising in the strain gradient theory. To demonstrate the capability of the proposed formulation in dealing with large deformations, specific examples involving an axisymmetric gradient shell structure subjected to severe circumferential load and a gradient plate are analyzed. The numerical results reveal that the deflections of a micro-scale shell predicted by the new model are smaller than those predicted by classical shell theory in the small and large deformation regimes.

Computational models and methods for predicting cancer progression and treatment response
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IN SILICO TRIALS INFORMED BY EXPERIMENTAL MEASUREMENTS REVEALS THE IMPACT OF PATIENT HETEROGENEITY ON DOSAGE PROTOCOL FOR A NOVEL CANCER THERAPEUTIC

Adrianne Jenner[*1]*

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ABSTRACT

Cancer growth and response to therapy varies significantly across the population. Immunotherapies have become an integral part of cancer therapy in recent years. Unfortunately, there is large variability in the responses of cancer patients to these therapies, including complete remission or rapid tumour growth. Bispecific T-cell engagers (BiTEs) are one promising immunotherapy that enhance cellular antitumour immunity by targeting T cells and priming them to recognize cancer cells. Recent evidence has suggested that BiTE efficacy can be heightened through encoding in oncolytic measles virus (MV-BiTE) vectors. Infection of cancer cells with MV-BiTEs causes the local production of BiTEs and has shown efficacy and safety in a murine model, however, the translated efficacy of this treatment in a heterogeneous human population is unknown. In this work, we generate an in silico clinical trial of MV-BiTE therapy in a cohort of heterogeneous virtual individuals informed by experimental measurements. Patients are generated through sampling parameters in an ordinary differential equation system based on variability in experimental measurements. Model predictions show there is a strong correlation between an individuals immune response and their response to this novel therapy. The methods developed here are easily translated to other cancer modelling areas, where understanding the impact of heterogeneity in patients is crucial.

Industrial applications of IGA
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GEOMETRICALLY WATERTIGHT UNSTRUCTURED SPLINES APPLIED TO CAD, FEA, IGA, CAM, AND CAI FOR A DESIGN-THROUGH-MANUFACTURING DIGITAL THREAD

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ABSTRACT

Currently, one of the Kansas City National Security Campus (KCNSC) initiatives is implementing a digital engineering approach that uses authoritative sources of data and models. A barrier to this approach is that computer-aided tools used in the design-through-manufacturing workflows (i.e., Computer-Aided Design (CAD), Computer-Aided Engineering (CAE), Computer-Aided Manufacturing (CAM), and Computer-Aided Inspection (CAI) etc., generically CAx) were initially developed independently, and as a result each domain utilizes a unique Model Based Definition (MBD) data model. Data consumed or generated in one CAx domain data model cannot always be accurately translated, consumed by, or associated with another CAx domain data model, severely limiting the degree to which any particular CAx domain data can be effectively linked to or leveraged by another domain. The fundamental way in which these CAx MBD data models are constructed severely limits the ability to perform isogeometric analysis (IGA) and update CAx geometry to create digital twins.
The root of this problem is that currently, native CAD models are not suitable for many of the requirements of the other CAx domains due to mathematical inconsistencies, such as non-geometric watertightness, that create problems for downstream users. This is due to inaccuracy of computing complex intersections of the non-uniform rational basis splines (NURBS) used in boundary representations (B-Reps), the de facto modeling description utilized by modern CAD systems, and means NURBS surface intersections must be represented as curve approximations. Thus, while CAD B-Rep definitions of geometry are topologically watertight, gaps of geometric discontinuity are introduced at these approximated intersections that do not allow them to be geometrically watertight.

KCNSC is partnering with nVariate, Inc. to address this by utilizing their patented watertight Boolean operation technology to create geometrically watertight models. These models consist of un-trimmed surface patches of explicit geometric continuity and can be accurate to the same model tolerance employed in existing CAD systems. The technology is implemented to produce watertight spline CAD models directly linked to traditionally authored CAD models in PTC Creo Parametric, the model authoring application at KCNSC. The watertight spline CAD model is used for improved workflows for finite element analysis (FEA) and IGA, creation of an improved digital twin model updated by analysis results, inspection data, and manufacturing data, and generation of improved slice files for additive manufacturing (AM).

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Advances in multi-scale, multi-material, and multi-component Topology Optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INTEGRATING MULTIPLE LOADING CASES IN HIGH-RESOLUTION TOPOLOGY OPTIMIZATION: A MULTI-SCALE APPROACH

Peter Dørffler Ladegaard Jensen[*1], Rebekka Varum Woldseth[1] and Ole Sigmund[1]*

[1]*Technical University of Denmark*

ABSTRACT

The seminal works on high-resolution topology optimization procedures have provided new insights into structural design [1]. Despite these advancements, their high computational costs limit practical industry applications. Concurrently, industrial-grade additive manufacturing (AM) has seen substantial improvements, highlighting the need for AM-specific high-resolution inverse design methods that integrate infill as a structural component.

These challenges were addressed by Jensen et al. [2] by extending the de-homogenization topology optimization method [3] to 3D unstructured grids, where a multi-scale optimization approach was employed by considering an orthotropic periodic rectangular-hole material, which is reminiscent of the stiffness optimal Rank-3 material. The microstructure orientations and laminates are regulated to enhance stability and manufacturability. The coarse multi-scale structure is reconstructed on a high-resolution single-scale by considering a finite periodicity of the microstructure, which corresponds to a minimum length scale, by computing stream surfaces that align with the microstructure, resulting in a high-resolution structure with a minor reduction in structural performance compared to the coarse scale optimized solution. However, this method was limited to a single-load assumption, resulting in suboptimal results if applied to multi-load scenarios. This work extends [2] by incorporating the optimal Rank-N microstructure as the material model, enabling the optimization of structures under multiple load-case scenarios. This advancement allows for the reproduction of complex structures like the wing study in [1], with significantly reduced computational resources and comparable structural performance.

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Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPERIMENTAL AND NUMERICAL STUDIES ON SHEAR BAND FORMATION AT HIGH STRAIN RATES

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ABSTRACT

The essence of dynamic failure is closely linked to dramatic shear deformations frequently resulting in the emergence of adiabatic shear bands (ASB). Under high loading velocities and the subsequent rapid temperature increase, the localization of shear strain is crucial in view of safety issues, especially with respect to fast rotating components and diverse crash scenarios. Therefore, we perform and numerically investigate high speed impact tests at the split Hopkinson pressure bar (SHPB) setup specifying notched hat-shaped specimen geometries that resemble the stresses and failure conditions at the component level.

First, using specimens manufactured from the steel S690QL and the nickel-based superalloy Inconel 718 we connect series of SHPB impact tests at high strain rates of 10^3-10^4 s^(-1) and quasistatic tests at rates of 10^(-3) s^(-1). Optical microscopy and electron backscatter diffraction (EBSD) unveil significant shear localization accompanied by grain refinement in the SHPB tests. Thus, the yield strength is doubled in the affected region which can be described by the Hall-Petch relation.

The displacements across the surface of the specimens are captured with subset-based local digital image correlation (DIC) during the impact time and combined with implicit and explicit finite element (FE) simulations to solve the inverse problem on the identification of the underlying viscoplastic constitutive model for finite deformations. More specifically, we identify the damage parameters of the widely recognized viscoplastic Johnson-Cook (JC) model with an enhanced description of the damage evolution. The temperature evolution is assumed to be adiabatic and compared with high-speed thermography measurements.

To ensure the well-posedness of the boundary value problem (BVP) we consider an extension by a nonlocal formulation. Therefore, we use the implicit gradient model approach formulated for the viscoplastic equivalent strain. Finally, we determine the additional internal length scale introduced by the gradient model from the inverse problem associated with the SHPB tests.

Multiscale computational and data-driven approach of advanced materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A REACTIVE MOLECULAR DYNAMIC SIMULATION STUDY ON HYPERTHERMAL EROSION OF BNNT BASED NANOCOMPOSITE UNDER LEO AND SUB LEO ENVIRONMENT

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ABSTRACT

Satellites and space vehicles aviating the LEO (Low Earth Orbit) are inevitably experience pyrolysis and ablation due to the collision with gaseous molecules and debris. Especially, under the LEO environment, atomic oxygen(AO) is the most abundant component of the atmosphere and causes a critical surface damage of thermal protection materials (TPM) for its high reactivity. In the sub LEO near 200~300km of altitude, however, the nitrogen molecule (N2) is as abundant as the AO. Therefore, the impact of these two main components should be considered in the design of TPM.
Boron nitride (BN) nanostructures such as hexagonal BN sheet and BN nanotubes (BNNT) are promising materials as reinforcement in TPM for their exceptional stability at elevated temperature. At the same time, BN nanostructures are highly conductive, stiff, strong comparable to the carbon nanotubes and possesses neutron absorption capability. Therefore, continuous attempts to utilize BNNT as coating materials for spacecrafts are being made.

In this study, a comparative hyperthermal bombardment simulation on the impact of AO and N2 in surface erosion of BN-based nanocomposites was performed using a reactive molecular dynamic simulation. The ReaxFF was adopted to describe the material's recession due to bond breaking in detail. Reflecting the atmospheric profile in sub LEO, AO and N2 were collided to the surface of polyimide (PI) and PI-BN nanocomposites with a kinetic energy of 4.5eV and 8.0eV, respectively for each component. To predict the ablation properties of PI-BN nanocomposite, the surface recession rate, temperature rising ratio by the AO and N2 were determined and compared with each other. Additionally, difference in the reaction products by the two components were predicted and discussed in conjunction with the recession ratio. Finally, erosion yield of PI and PI-BN nanocomposites were determined according to the ratio of colliding AO and N2 and compared with MISSE experimental results.

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Advances in damage & fracture modeling of multiphysics materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFECT OF TANGENTIAL FRACTURE PROPERTIES ON MIXED-MODE COHESIVE ZONE MODELING

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ABSTRACT

Determining tangential fracture properties poses significant challenges, particularly in solving mixed-mode problems. Thus, most previous researchers simply focused on the normal cohesive fracture properties while either neglecting the tangential traction with a low stiffness or assuming the same traction-separation relation as the normal one. To investigate the effect of tangential fracture properties on mixed-mode cohesive zone modeling, the Park-Paulino-Roesler (PPR) model (Park et al., 2008) is employed and modified (Jeon and Park, 2024). The original PPR model provides both normal and tangential cohesive traction-separation relations in conjunction with corresponding fracture properties, while displaying a tangential traction discontinuity at zero separation in the extrinsic cohesive zone modeling. The extrinsic PPR model is modified through removing the tangential traction discontinuity with an initial elastic region only for the tangential traction. Then, three mixed-mode examples, i.e., mixed-mode bending test, semi-circular bending test, and four-point shear test, are simulated using the modified PPR model in conjunction with stress recovery and domain integral (Choi and Park, 2019). The computational results demonstrate the significant effects of tangential fracture properties on load-displacement responses. Furthermore, this model is anticipated to have broad applications across various mixed-mode failure scenarios, taking into account the effects of normal and tangential fracture properties.

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Physics-informed machine learning for numerical modelling in engineering and science
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NOVEL TOPOLOGY OPTIMIZATION FRAMEWORK USING PHYSICS-INFORMED NEURAL NETWORK

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ABSTRACT

To this date, Deep Learning (DL) data-driven methods have been successfully applied to various topology optimization problems where DL models are trained to establish a mapping between the optimized topology with corresponding boundary conditions. Such method has inherent drawbacks, where the DL model requires a large training dataset to train and yet is challenged due to the poor generalization of their models. Therefore, mitigating the reliance on data while demonstrating superior generalization ability is highly desirable. The present study introduces a novel DL-based computational paradigm for topology optimization by leveraging the Physics-Informed Neural Networks (PINNs) that can be trained without labelled data to solve computational physics problems while respecting the laws of physics in the format of Partial Differential Equations (PDEs) [1]. In our proposed framework, we employ the Deep Energy Method (DEM) to numerically calculate the displacement field of the given problem domain by minimizing the overall potential energy as the natural loss of the PINN [2]. Subsequent sensitivity analysis is carried out using the automatic differentiation feature in DL to solve the derivative of the objective function with respect to the network parameters [3]. The numerical examples demonstrate that the proposed framework is capable of solving various topology optimization problems without facing any generalization issues for compliance minimization, stress-constrained and three-dimensional problems. In particular, the resulting designs exhibit comparable objective values to the designs obtained via Solid Isotropic Material with Penalization (SIMP) method.

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Minisymposium in honor of Prof. Yannis Kallinderis's 60th birthday: Progress of Unstructured grid based CFD, hybrid mesh generation and adaptation, and parallel supercomputing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NUMERICAL ANALYSIS OF PPTC2 PROPELLER OPEN-WATER CHARACTERISTICS USING DISCONTINUOUS GALERKIN METHOD

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ABSTRACT

This paper introduces the unstructured grid-based incompressible flow solver, ULSAN3D-Unstr and presents the numerical analysis results of the propeller open-water characteristics of the PPTCⅡ-P1727 tip-rake propeller developed by SVA Potsdam. ULSAN3D-Unstr employs Discontinuous Galerkin Method and for discretize Incompressible Navier Stokes equation. In order to the treat incompressiblity fluid flow, Artificial Compressibility Method is used and calculates flow fluxes using Upwind schemes, enabling much stable flow analysis. The fluid flow around the propeller is simulated using the Multiple Reference Frame (MRF) approach, and pseudo-time stepping to a steady-state is conducted using an Implicit Method, allowing for dramatical convergence without constraints on time advancement. Through a numerical analysis of PPTCⅡ Propeller Open-Water Characteristics propeller, the paper aims to figure out rake performance which reduce vortex shedding behind the propeller blades of the PPTCⅡ and validate the accuracy of unstructured grid-based incompressible flow solver, ULSAN3D-Unstr.

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Physics-based data-driven modeling and uncertainty quantification in computational materials science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MODULAR NONLINEAR STOCHASTIC FINITE ELEMENT FORMULATION FOR UNCERTAINTY ESTIMATION AND PARAMETER SENSITIVITY ANALYSIS

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ABSTRACT

The Monte Carlo method has been widely used for the uncertainty estimation in mechanical engineering design. While extremely flexible, this method remains impractical in terms of computational time and scalability. To circumvent these limitations, other approaches such as the Galerkin stochastic finite element method (GSFEM) have been proposed. GSFEM, pioneered by Spanos and Ghanem [1], provides accurate statistics of the output, has the advantage of being sampling-independent and can be modular in terms of operations, albeit code intrusive. While linear elasticity has been extensively covered in the literature, the application of GSFEM to nonlinear mechanical behaviour remains relatively unexplored. Here, we proposed a formulation of GSFEM that i) makes use of a hybrid formulation to capture discontinuous behaviours [2], ii) allows for nonlinear behaviour, and iii), by special consideration of the input distribution, allows for parameter sensitivity analyses [3,4].

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Advanced computational modelling of wood, wood-based products, bio-composites, and timber structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THERMAL CONDUCTIVITY OF NANOPAPER FILMS: A CONTINUUM MICROMECHANICS APPROACH

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ABSTRACT

Nanopaper films made of cellulose nanofibrils are suitable candidates for heat management in several flexible electronics applications [1]. However, natural, as well as technical and technological variability, often results in nanopaper films exhibiting a wide range of thermal properties. Hence, it is important, from an application viewpoint, to develop theoretical models that can guide empirical activities related to such materials (such as their production, research and development, or use), and assist in reducing present uncertainties. With this purpose in mind, the mathematical analogy, in the context of continuum micromechanics and mean-field homogenization, between the conductivity and the elasticity problems [1], serves as starting point for adaptation of a continuum-micromechanics-based theoretical model for the elasticity of paper sheets, to the case of thermal conductivity of nanopaper films [1]. Thereby, large collections of experimental determinations are used to compute volume fractions of crystalline cellulose Iα, crystalline cellulose Iβ, crystalline cellulose II, amorphous cellulose, and water in “mean” cellulose nanofibrils of various origins [2]; while a selection of thermal conductivity properties of the abovementioned constituents of nanofibrils, enables estimation of respective thermal conductivity tensors [1]. It is important to note that the thermal conductivity of hydrated amorphous cellulose (the material that indeed embeds the cellulose crystals), as a function of water content, is not directly available; and that, satisfaction of separation of scales conditions formally excludes self-consistent homogenization of amorphous cellulose and water, leaving only atomistic or sub-atomistic approaches available. As a remedy, we resort to recent findings on the elasticity of cellulose nanofibrils [2] and employ Mori-Tanaka homogenization of cellulose crystals and water, embedded into a dry, amorphous cellulose matrix, to estimate a reliable thermal conductivity tensor for the corresponding composite. Theoretically predicted relationships between porosity and in- as well as out-of-plane thermal conductivity of corresponding nanopaper films, agree well with respective, experimentally determined relationships [1]. Similar agreement is found for cellulose fibrils [1]. The proposed theoretical model gives access to similar models (for instance, for water diffusivity or permeability), and paves the way to a higher level of control in empirical activities related to such materials.

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Emerging topology and shape optimization techniques in computational design of materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPARING TOPOLOGY-OPTIMIZED REINFORCED CONCRETE BEAMS DESIGNED WITH 0-1 AND VARIABLE THICKNESS METHODS

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ABSTRACT

Topology optimization (TO) is a design optimization method known to generate high-performing structures with a limited volume of material. TO is particularly powerful because it does not require an initial layout of structural members from the user. Rather, it places material freely inside a defined design space with known forces and boundary conditions, so the method can algorithmically derive highly efficient results. TO has enormous potential for impact in the construction industry because it can help reduce the use of building materials, which produce approximately 10% of greenhouse gasses worldwide [1].

Within existing research on TO for construction, tailoring algorithms specifically to reinforced concrete (RC) design has received considerable attention [2]. RC is an important structural system for research because it is ubiquitous in the construction industry. It can also be easily formed into shaped molds, allowing it to be adapted to complex optimized geometries. A common approach for TO of RC uses continuum elements that are stiff in compression to represent the placement of concrete struts, and truss elements that are stiff in tension to place steel ties. These two components come together to create a truss-like RC structure following the strut-and-tie method [3].

This research will present a new framework for topology optimization of RC. Continuum and truss elements will be used together as in [3], but the locations of the nodes of the truss elements will be controlled by design variables, and able to move during the optimization process. Also, SIMP penalization schemes will not be used on the continuum elements, so that their respective design variables can take intermediate values between 0 and 1. These values will be interpreted as varying thicknesses in the final design, following the Variable Thickness Sheet method. Several numerical design examples will be presented using this new framework, and mid-scale designs (~1 meter spans) will be fabricated and tested to demonstrate their efficacy.

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Biomechanics of hard tissues: From experiments and simulations to clinical applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INFLUENCE OF SOFT TISSUE THICKNESS ON THE SIDEWAYS FALL MODELS

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ABSTRACT

Trochanteric soft tissue thickness (TSTT) is an important factor influencing the probability of a fracture of the proximal femur following a fall [Pretty et al.,2021, Fleps et al., 2019]. To build personalized biofidelic finite element models (FEM) of human hips, we collected whole body DXA scans using Hologic® Horizon W scanner and body shape (optical) scans using TC2® scanner for 188 subjects (109 Females, 79 males). One of the challenges of accurately determining the TSTT from the whole body DXA scans is associated with the fact that the subjects are scanned in supine position which leads to overestimation of the TSTT as the tissue over the greater trochanter (GT) region is pushed outwards due to the subject's body weight. To address this, we developed a novel method which corrects TSTT based on the optical scans. Briefly, this method utilizes open-source python (v3.9.x) packages to measure TSTT from the two scan sources. The average TSTT (TSTT_avg) of both sides was used to minimalize the measurement error due to preferred weight shifting by the subject during the scan. The TSTT in the supine position (DXA scan: TSTT_avg_scanned) and the standing position (optical scan: TSTT_avg_corrected) was compared for the respective 188 subject's body mass index (BMI) and the correction equation was obtained (eq. 1). The scanned and corrected hip width (HW_scanned, HW_corrected) are obtained from eq. 2 & 3.
TSTT_avg_corrected = 0. 6843 x TSTT_avg_scanned - 0.5461 – (eq.1)
HW_scanned = ΔGT_Left&Right + [2 x Avg. (TSTT_avg_scanned)] – (eq.2)
HW_corrected = ΔGT_Left&Right + [2 x Avg. (TSTT_avg_corrected)] – (eq.3)
where, ΔGT_Left&Right = Distance between left and right greater trochanter point (lateral most).
To demonstrate the influence of this correction we subjected 25 biofidelic FEM to a simulated sideways fall at an impact speed of 3.1 m/s. The soft tissue for the biofidelic FEM creation is selected based on subject's gender, hip width, weight, and BMI. Scanned and corrected hip width were used for each subject to create respective models. The number of hip fractures, determined using a strain-based criterion, increased from 11 to 20 after the correction. The average increase in predicted femur force (17.47%), impact force (6.41%) and drop in force attenuation (11.87%) were recorded. Thus, to generate biofidelic FEM for assessing hip fracture risk due to sideways fall, it is critical to correct TSTT measured in supine position.

Multiscale modeling, analysis and numerical methods of material defect and inhomogeneities
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE MODELLING OF DEFECT KINETICS IN IRRADIATED ZR-SN-NB ALLOYS

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ABSTRACT

The development of fuel cladding material is a core technology that crucially affects nuclear power plants' safety, reliability, and economy. Due to their excellent performance, Zr-Sn-Nb alloys have become the mainstream of future cladding material development. During service, Zr-Sn-Nb alloys are subjected to strong neutron irradiation and high temperature, which significantly changes their microstructure and mechanical properties, resulting in performance degradation such as irradiation growth, seriously threatening the safe operation of nuclear reactors. However, due to the anisotropy and temperature-dependent behaviour of Zr alloys and the complex effects of alloying elements addition, the microstructure evolution and irradiation growth behaviour of Zr-Sn-Nb alloy under irradiation are far from clear.

This work established a systematic cluster dynamics and dislocation dynamics model for modelling defect evolution and predicting the irradiation growth of Zr-Sn-Nb alloys. The model considers the temperature dependence and anisotropy of Zr alloys, and reasonably handles the effect of various alloying elements. The simultaneous evolution of point defects, small defect clusters, and microstructures including dislocation lines and irradiation loops on the prismatic and basal plane, as well as Nb-induced precipitates in Zr-Sn-Nb alloys is obtained. Results of defect density, size and irradiation growth strain from the model and experiments of Zr, Zr-Sn, Zr-Nb and Zr-Sn-Nb alloys are compared and all in good agreement, verifying the proposed model. Based on the model, the effect of Sn and Nb on microstructural evolution and mechanical properties of Zr alloys is evaluated. Further, the irradiation temperature range of 473-673K is studied, which covers the service temperature range of cladding material in the widely used pressurized water reactor and boiling water reactor.The proposed model provides a powerful tool for developing new cladding materials.

Recent advances on interfaces dynamics modeling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DROPLET COALESCENCE ON A SLOPED CYLINDRICAL WIRE

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ABSTRACT

Transporting droplets along cylindrical wires is an emerging focus area with various practical applications such as fog collection and filtration. Recent experiments by Feng et al. (2022) have revealed a wealth of new droplet coalescence dynamics on a superhydrophilic cylindrical wire, illustrating the need for more advanced theory. In this study, we present a mathematical model using lubrication theory and weighted residual modeling techniques for a thin liquid film flowing on a tilted superhydrophilic cylinder. This model incorporates key physical factors such as gravity, low-to-moderate inertia effects, surface tension, and disjoining pressure. This model explains the observed phenomenon of directional self-propelled transport during droplet coalescence, where the large droplet moves towards the small one. Moreover, we identify two distinct coalescence modes that result in either droplet oscillations or quasi-static droplet collapses. Stability analysis and numerical simulation agree well against the experimental observations.

TOPOLOGY OPTIMIZATION OF THERMAL MANAGEMENT SYSTEMS WITH CONTROL STRATEGIES

Yonghwa Ji[*1] and Jaewook Lee*[1]

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ABSTRACT

Efficient thermal management systems are increasingly vital in the context of electrified mobilities, impacting key components such as batteries and electric motors [1]. Liquid cooling, a widely adopted approach for electrified mobilities, necessitates the design of efficient cooling channels to maximize cooling capacity while minimizing pressure drop. To determine the optimal geometry for enhanced performance, topology optimization has been applied to various fields including structural mechanics, heat transfer, and fluid mechanics [2]. Topology optimization based on the conjugate heat transfer phenomenon has proven effective at the single-part level in prescribed boundary conditions [3]. However, a critical gap exists in the analysis of thermal management system performance under varying conditions, as existing studies only consider prescribed boundary conditions. Consequently, comprehensive evaluation of thermal management system performances requires the incorporation of control strategies to address dynamic environments.

This research aims to validate the enhanced performance of thermal management systems by integrating topology optimization results with control strategies, employing exergy analysis based on the second law of thermodynamics. A cooling channel that maximizes both heat transfer and fluidic performance is designed through the utilization of a multi-objective topology optimization approach. Exergy analysis is facilitated by surrogate models based on machine learning, enabling the calculation of thermal management system performances. The comparison of thermal management systems is conducted between a thermal management system with conventional components and one incorporating components derived from topology optimization.

Acknowledgement

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Advances in damage & fracture modeling of multiphysics materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NOVEL DUAL LATTICE DISCRETE PARTICLE MODEL FOR MULTIPHYSICS SIMULATION OF COUPLED MECHANICAL AND TRANSPORT BEHAVIOR IN CONCRETE MEMBERS SUBJECTED TO LONG-TERM LOADING

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ABSTRACT

Chloride ingress is a critical cause of reinforcement corrosion in structural concrete. In coastal and snow-belt areas, concrete members are continuously exposed to seawater and deicing salts, which are rich in chloride ions. Driven by water convection and diffusion of ions, chloride migrates into the concrete and gradually reaches the reinforcement. The presence and evolution of microcracks caused by external loads also promote faster intrusion of chloride ions from the surface to the rebars. Under long-term loading, cracking can be further exacerbated by creep, leading to an acceleration in chloride transport. In this context, effective corrosion prediction requires multi-physics modeling strategies, considering both chloride transport and load-induced cracking. However, most current models focus on prescribed cracks and ignore the long-term effects of sustained loads on crack propagation. This work proposes a dual lattice discrete particle model (LDPM) for the simulation of coupled fracture, creep and water-chloride transport. The dual LDPM inherits the advantages of LDPM in simulating concrete fracture, including viscous effects. The water-chloride transport element is then established by exploiting the duality between the Delaunay tetrahedralization and LDPM tessellation. To express the influence of cracking on chloride ingress and mass transport, a nonlinear formulation between mesoscale crack width and effective diffusivity is formulated. Solution for the coupled model is implemented by means of two different strategies. Fracture and creep performance are analyzed using a dynamic explicit solver with central difference scheme, while water and chloride transport are resolved by a dynamic semi-implicit scheme employing Crank-Nicolson and Newton-Raphson solvers. The dual LDPM is calibrated and validated by comparing simulation results with reported tension, compression, and three-point bending experiments available in the literature. Results demonstrate the capability of the proposed dual LDPM in predicting chloride ingress in concrete members subjected to different damage levels under both short- and long-term loading conditions.

Uncertainty quantification and reliability analysis in engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SOIL-STRUCTURE INTERACTION EFFECTS IN SEISMIC FAILURE PROBABILITY ANALYSIS OF BRIDGES WITH MULTIPLE LOAD COUPLING

Mingming Jia[*1] and Yijiang Wan*[1]

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ABSTRACT

Soil-structure interaction (SSI) has a significant impact on the performance of large-scale bridge structures in multi-layered soils, especially under strong ground motions. Quantifying the uncertainty can provide support for structural failure probability analysis. Considering SSI effects in an experimental setting involves cumbersome procedures that are difficult to control and monitor. At present, there are only the Winkle foundation method and the finite element method in numerical models, which makes it hard to balance accuracy and computational efficiency. Therefore, it is essential to develop a new machine learning-assisted numerical method to accurately and efficiently quantify SSI uncertainties. The purpose of this study is to analyze the SSI effects of bridge failure probability under strong ground motions. Focusing on the pile-supported piers, the structure is a single-column group-piles system, connected with the superstructure simply supported. The pile group is anchored to a robust bedrock and comprises end-bearing piles. The Monte Carlo method is used for modeling analysis of multi-layered soil strength uncertainty, structural material uncertainty, and pile-soil contact uncertainty. The linear elastic properties and radiation damping of far-field soil, the plasticity of near-field soil, and the sliding and debonding process of the pile-soil interface are extracted by the cyclic neural network. On the other hand, the time-history characteristics of the inertia load of the superstructure are captured. The failure probability of the pier structure is judged based on the multi-load coupling failure theory.

Battery modeling and computation: From material to device
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MATHEMATICAL MODEL FOR THERMAL RUNAWAY PROPAGATION WITHIN CELLS

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ABSTRACT

Thermal runaway (TR) is one of the dangerous failure modes of lithium-ion batteries (LIBs). In real situations, thermal runaway is commonly initiated within a local heat point and propagates to the entire cell. The propagation behavior, such as front and velocity, determines the energy released rate and temperature distribution. Therefore, it is of great importance to describe thermal runaway propagation efficiently and accurately. Recently theoretical and experimental research indicated that thermal runaway propagates within cells with a around constant velocity. The velocity is also found to be related to the reaction rate and thermal conductivity. In this work, we further investigate more general cases that consider the anisotropic and jellyroll structure of cells. Our theoretical derivation shows that the thermal runaway propagation velocity will also tend to be a constant value when the front is far away from the initial heat source. The theoretical propagation velocity and propagation front were derived. The results are validated both by numerical simulation and TR triggering tests of commercially used 18650 cylindrical cells from the NERL Battery Failure Databank. The theoretical front shape is consistent with experiment speculation. Based on this theory, the energy release rate during the TR propagation was discussed. Cells would have the highest energy release rate when their normalized dimensions were proportional to the thermal conductivity in the corresponding directions. Furthermore, the effect of preheating is discussed based on the hypothesis of point heat source and infinite space. In this case, the TR propagates with the maximum velocity first and quickly convergence to a stable lower value. The results will provide insights for thermal runaway modeling and safety design.

Computational mechanics of soft matter and machines
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ANOMALOUS FRACTURE BEHAVIOR OF SOFT LAYERED MATERIALS

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ABSTRACT

Soft layered material systems are ubiquitous in nature and engineering – from natural biological tissues to engineered devices. However, from the mechanics perspective, why soft layered materials are favored by natural selection and engineering design remains largely unexplored. Here we study the fracture mechanics of heterogeneous soft layered materials. We develop a theoretical framework for analyzing the co-evolving channel cracking and interfacial delamination in soft film/substrate systems, which is then applied on investigating the fracture of bilayer hydrogels – a representative soft layered material. Through both experiment investigation, theoretical analysis and numerical modeling, we find that the heterogeneous soft layered materials exhibit anomalous size-independent fracture behaviors with fracture strains independent of the flaw size and overall structural dimensions, in stark contrast to ordinary homogeneous materials whose stretch at break reduces undesirably with increasing flaw size and structural dimensions. The size-independent fracture behavior leads to notable toughening of soft layered materials. The findings hold for a broad range of hyperelastic soft materials, from biological materials to hydrogels and elastomers, opening potentially new avenues for the development of fracture-resistant soft materials, and motivating new investigations of the development and applications of heterogeneous soft materials.

Catastrophic failure mechanics and numerical modelling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STUDY ON THE ANNEALING BLISTERING BEHAVIOR OF IRRADIATED U-10MO/AL MONOLITHIC FUEL PLATE

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ABSTRACT

U-10Mo/Al monolithic fuel plate is composed of U-10Mo fuel foil, Al alloy cladding and Zr diffusion barrier layer, which has delightful application prospects in the research and test reactors due to its high uranium density and stable irradiation performance under normal conditions. It is very important to ensure its safe operation under accident conditions. The blister threshold-temperature obtained by the annealing experiments on the irradiated fuel plates, can be utilized to test the ability of the fuel plated under accident conditions. Compared to the experimental methods, which are expensive and time-consuming, it is an economical and efficient approach by utilizing numerical simulation techniques to study the annealing blistering behavior of U-10Mo/Al monolithic fuel plates combining experimental data.

The annealing experiments of U-10Mo/Al monolithic fuel plates indicate that the blistering behavior of fuel plates is closely related to their irradiation history, which is thermal-mechanical coupling behavior. As the nuclear fission progresses during irradiation, fission gas is generated inside the U-10Mo fuel grains, forming and growing the fission gas bubbles at the grain boundaries, leading to a pressurized porous structure of U-10Mo fuel foil. The fission gas swelling is related with the temperature and macroscale hydrostatic pressure. The material properties of U-10Mo fuels including the elastic constants, thermal conductivity and materials strength will be degraded owing to the porosity and the irradiation damage. The temperature changes during the annealing process cause both thermal stress and pore pressure variations of the U-10Mo fuel foil, and the thermal creep behavior of cladding. The crack will occur in the U-10Mo fuel foil with the interaction of fuel foil and cladding, and pore pressure. A cavity pressure will take place due to the release of fission gas atoms, accelerating the propagation of cracks. The macroscale deformation of Al alloy cladding will happen with the effect of temperature and cavity pressure, resulting in the local blistering behavior.
In this study, a three-dimensional incremental constitutive relationship will be established comprehensively considering the thermal-mechanical properties for the whole irradiation-annealing process. A cohesive zone model considering the porosity effect will be developed to describe the initiation and propagation of cracks for U-10Mo fuels, together with the coupling model of fission gas release-volume-cavity pressure. The blistering behavior of U-10Mo/Al monolithic fuel plates will be analyzed, and the underlying annealing blister mechanism of fuel plates will be revealed.

Advances in numerical methods for solution of PDEs
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STATE SPACE BASED MIXED FINITE ELEMENT METHOD FOR LAMINATED STRUCTURES

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ABSTRACT

Laminated structures are widely used in various engineering fields. Using combination of different materials, they can achieve excellent mechanical characteristics, such as high strength-mass ratio and adjustable stiffness. Numerous methods are therefore proposed to analyze their mechanical performances [1]. However, as elastic modulus and Poisson's ratios are different across the thickness direction, shear deformation distributions become complex and it requires high-order shear deformation theories to give accurate displacement predictions for those laminated structures. The state space method is suitable for composite structures with arbitrary multiple layers. It preserves both displacement and stress continuities across the thickness direction. But it requires simple material distribution and loading conditions on other directions, which limit its applications. In order to make this method more flexible, finite element discretization on those directions are introduced in this paper, with nodal displacements and their energy-conjugated stresses as state variables, which conveniently handles continuity requirements and various transfer characteristics at the interfaces. The differential quadratic method (DQM) is further introduced to improve calculation stability.

Under such framework, static and dynamic behaviors of partially-connected composite beams are analyzed. The analyses of interlayer slip, stress distributions and natural frequencies of composite beams under different support conditions, loading arrangements and span combinations verify the correctness of the present method. Based on finite element meshing, non-uniform shear stiffnesses can be set along the longitudinal direction between layers to simulate spaced studs connection, which shows the advantage of this method to consider detailed structure configurations [2].
As finite element method provides flexibility for various boundary conditions and arbitrary in-plane shapes, laminated plates are further analyzed. Displacement and stress distributions of simple-supported laminated plates are analyzed and verified. Other boundary combinations of clamped and free edges are also calculated. Zero shear stress distributions on free boundaries are accurately satisfied using this method, and the calculation cost is significantly low comparing to ANSYS. Analyses of irregular plate shapes with holes on opposite sides shows geometric flexibility of the present method, and influences of holes on stress redistributions are clearly and accurately demonstrated.

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Computational mechanics of soft matter and machines
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FINITE ELEMENT SIMULATION ON INSTABILITIES OF DIELECTRIC ELASTOMERS CONSIDERING NONLINEAR MATERIAL VISCOSITY

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ABSTRACT

Dielectric elastomers (DEs) have attracted great research interests due to their unique features such as softness, flexibility, large deformation capacity and electromechanical coupling properties. However, the applications of DE-based devices have been limited by various potential instability modes including electromechanical instability (EMI) and some other stimuli-induced structural bifurcations. When undergoing large deformation, DEs exhibit nonlinear material viscosity, which makes it more challenging to accurately predict their instabilities. To fill this research gap, a finite element (FE) framework is developed to investigate the electromechanical responses and different instability modes of DE structures with the implementation of the nonlinear field theory and a micro-macro constitutive model that incorporates the deformation-dependent material viscosity. A highly customized user-element subroutine (UEL) in Abaqus is developed for the FE implementation. The material viscosity is modeled to be dependent on the global deformation based on a tube model derived from polymer dynamics. On this basis, the effects of nonlinear material viscosity on different instability modes of VHB 4910 structures are investigated, and the simulated results are compared with existing experimental data and analytical studies to validate the accuracy and robustness of the proposed model. This work provides a general approach for instability analysis of DE actuators with different configurations and can further function as a universal platform for numerical analysis on the electromechanical finite deformation of DE structures with complex configurations, leading to better design and applications of DE-based devices.

Advances in material model calibration for computational solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IDENTIFYING MATERIAL PARAMETERS OF PRINCIPAL STRETCH-BASED HYPERELASTIC MODELS WITH THE VIRTUAL FIELDS METHOD

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ABSTRACT

This work deals with parameter identification of principal stretch-based hyperelastic materials using the reformulated virtual fields method (VFM) based on the variation of elastic energy. Traditional VFM framework calculates the internal virtual work (IVW) as a product of one of the three types of stresses (Cauchy stress, the first Piola–Kirchhoff stress, or the second Piola–Kirchhoff stress) and its corresponding conjugate virtual strain, which often involves intricate mathematical derivations and computations. For example, the traditional method requires solving the hydrostatic pressure to obtain the first Piola–Kirchoff stress for incompressible materials [1], introducing an additional layer of complexity. In this study, we develop a reformulated version of VFM termed variation-of-elastic-energy-based virtual fields method (VEE-VFM), where the IVW is considered as the variation of elastic energy caused by virtual displacements, eliminating the need to calculate stress and its conjugate virtual strain [2]. The VFM is reformulated by calculating the IVW through the variation of elastic energy, which is more concise and easier to implement. In the reformulated VFM, an important step in calculating the IVW of principal stretch-based hyperelastic models is the calculation of the variations of principal stretches. Two approaches are proposed in this work: 1) the variations of principal stretches are directly correlated to the virtual deformation gradient based on the chain rule; 2) alternatively, we compute the variations of principal stretches by solving a system of linear equations which are constructed based upon the relation between the invariants and the principal stretches. To illustrate this reformulated framework and the proposed methods of calculating the variation of principal stretches, the first-order Ogden model is selected for this study, and numerical biaxial tensile experiments which give rise to heterogeneous deformation fields are performed on this type of material. Finally, material parameters are successfully extracted using the reformulated VFM framework, and the accuracy and robustness of VEE-VFM are demonstrated through simulated experiments, highlighting its reliability even in the presence of noise.

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Advances and applications of polytopal methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN ALGORITHM BASED ON THE SCALED BOUNDARY FINITE ELEMENT METHOD AND DEEP LEARNING FOR THE IDENTIFICATION OF MULTIPLE CRACKS IN MASSIVE STRUCTURES

Shouyan Jiang[*1], Wangtao Deng[1], Ean Tat Ooi[2], Liguo Sun[1] and Chengbin Du[1]*

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ABSTRACT

Structural defect identification is a vital aspect of structural health monitoring used to assess the safety of engineering structures. However, quantitatively determining the dimensions of structural defects is often difficult. Therefore, this study presents an innovative data-driven algorithm that combines the scaled boundary finite element method (SBFEM) and a deep learning framework based on a dilated causal convolutional neural network (CNN) to identify crack-like defects in large-scale structures. The SBFEM is used to simulate different crack-like defects. Mesh generation is significantly simplified by a simple procedure that requires only changing the scale centre at the crack tip and the positions of the nodes at the crack opening. This minimises remeshing and enables simple generation of sufficient data to train the neural network. In addition, an absorbing boundary model based on Rayleigh damping is used to avoid computing the entire model when simulating wave propagation in massive structures. To ensure that sequential data remain ordered and to obtain a large receptive field without increasing the complexity of the neural network, a dilated causal CNN is employed in the deep learning framework. Therefore, more historical information is captured, and the complex mapping relationship between the echo signal and the crack information is efficiently learnt. The proposed model can accurately identify the number, location, and depth of cracks in massive structures. Moreover, it is robust to noise, which is demonstrated via numerical examples. Therefore, the proposed algorithm provides valuable insight into the detection and diagnosis of structural defects, which can ultimately improve the safety of engineering structures.

Computational and analytical advances in nonlocal modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFICIENT NONLOCAL-TO-LOCAL COUPLING

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ABSTRACT

In this talk, we propose a non-intrusive and simple "splicing" method for local-to-nonlocal (LtN) coupling with variational methods. This is in contrast to the established splicing approaches of using particle methods. Furthermore, we rigorously show that our approach is in fact equivalent to a optimization-based LtN coupling method, and inherits many valuable theoretical properties such as convergence while still being cheap to solve.

Computational mechanics in Canada and China: Current states of shared scientific interests and opportunities for the future cooperation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTATIONAL MODELING OF TRANSPORT PHENOMENA IN FLUIDS AT SMALL SCALES

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ABSTRACT

Transport phenomena in fluids at small scales play vital roles in science and engineering. Numerical modeling and fundamental understanding of these phenomena are crucial for improving performance of technologies in areas such as biology, medicine, and energy storage, to name a few. This talk will discuss recent research progress made in the Micro/nanofluidics Group at Institute of Mechanics, Chinese Academy of Sciences. The topics we worked on include particulate transport in low-Reynolds-number fluids under general geometries, ionic transport in room-temperature ionic liquids in confined and unconfined spaces, and contact angle hysteresis at electrified ionic liquid-solid interfaces. Computational tools used to investigate these transport phenomena will also be discussed. Our research reveals that hydrodynamic interaction, electrostatic interaction, ion-ion correlation, and the structure and energetics at interfaces are main factors of the observed phenomena. In the end, we will discuss future research interests and possible opportunities to explore collaboration.

The phase field method for fracture: Theory, numerics, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A UNIFIED STRAIN ENERGY DECOMPOSITION STRATEGY UNDER THE LOCAL COORDINATE SYSTEM FOR PHASE FIELD FRACTURE MODELING

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ABSTRACT

The various currently existing phase field decomposition approaches exhibit efficacy in capturing mechanical behaviour within their preferred stress state regions. This study aims to propose a novel unified phase field decomposition model capable of appropriately decomposing strain energy across arbitrary stress states. The total strain energy is decomposed into three non-negative components, namely tensile, shear and compression parts on the local coordinate system (LCS) considering the Poison effect. The LCS is determined by the three normal stresses on it to achieve the maximum F-function energy, which drives the fracture propagation in this model. This local coordinate system decomposition (LCSD) model could recast to the common-adopted spectral, V-D and crack-surface-based strain energy decomposition strategies for specific stress state regions, which has proven to be related to the ratio between shear and tensile crack energy release rate as well as the Poison ratio. Furthermore, a unified strength criterion is incorporated for the update of the LCS to ensure the stability of the original damaged surface. The proposed model is implemented via ABAQUS explicit code with VUEL and VUMAT subroutine. Verification of this proposed LCSD phase field model is conducted by comparing its simulation results with the isotropic, spectral and V-D decomposition model through a comprehensive series of numerical examples, encompassing uniaxial tension and compression test on the dogbone specimen, triaxial compression test on the pre-cracked cylinder specimen and the perforated asymmetric bending test, which cover various stress states including tension, compression, shear-compression and shear-tension stresses. Additionally, the performance of this model under dynamic loading is also validated through the renowned Kalthoff–Winkler impact test.

Emerging topology and shape optimization techniques in computational design of materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION DESIGN OF UNDERWATER PRESSURE HULL FOR SUBMERSIBLE

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ABSTRACT

As the key component of submersible, the design of underwater pressure hull is particularly important. In this work, based on a parameterized level-set method using radial basis functions, a topology optimization method is proposed that can account for the design of underwater pressure hull for submersible. The optimal design of underwater pressure hull is studied by using the buoyancy factor minimization as the objective function, the critical buckling factor and the yield strength as the design constraint. To provide clear and continuous mathematical expressions for the normal velocities, the theory of the shape derivative and bifurcation analysis are used to obtain the normal velocities in the parameterized level-set method, and we propose an easily implemented method to discretize normal velocities to every nodal point in the design area. An augmented Lagrange multiplier is given to realize stable transitions of both optimization problems during the convergence process. The effectiveness of the proposed method is validated by numerical examples, and it has engineering application value for the exploration of new underwater pressure hulls.

Advances in computational biomechanics and mechanobiology
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A COMPUTATIONAL STUDY OF THE INFLUENCE OF CARDIAC MECHANICS IN DESMOPLAKIN CARDIOMYOPATHY

Javiera Jilberto[*1], Renee Miller[2], Adam Helms[1] and David Nordsletten[13]*

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ABSTRACT

Desmoplakin Cardiomyopathy is a genetic disease that compromises the sub-cellular structure responsible for mechanically linking cardiomyocytes. Unlike other cardiomyopathies, patients with this disease present a unique pattern of fibrosis that focalizes in the subepicardial layer of the left ventricle (LV) [1]. The heterogeneous mechanical loading of the left ventricular wall is thought to be responsible for this pattern. To investigate this hypothesis, we use image-based biomechanical modeling to build a virtual cohort of patients (n=17) with different levels of disease severity. The models are generated using a modification of a previously developed pipeline [2], which uses machine learning and image processing tools to extract structural and functional data from magnetic resonance images (MRI) of the patients' hearts. In this pipeline, we also implemented a process to identify fibrotic areas from late gadolinium enhancement MRI. This information is merged into the biomechanical models using universal ventricular coordinates [3]. By analyzing the data of the virtual cohort, we define the trends of LV wall thinning, fibrotic patch increasing, and the changes in pressure and volume traces.

To understand how mechanics are related to the observed disease progression, we used a healthy patient geometry as a baseline and simulated the mechanics for five stages of disease severity. The myocardium is modeled using a Holzapfel-Ogden model, with the fibrotic patch being stiffer and non-contractile. We utilize a data-assimilation process [2] to estimate the cardiac activation levels given the pressure-volume loop. Mechanical quantities such as strain, strain rate, and stress are quantified and correlated with the spatial maps of fibrosis. We observe that strain and strain-rate values are exacerbated in the subepicardium, especially during isovolumic contraction, and the presence of fibrosis exacerbates the mechanical loading of neighboring areas. This study provides a comprehensive investigation of how mechanics are related to the progression of Desmoplakin Cardiomyopathy and provides key knowledge that can help clinicians design better treatments for these patients.

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METAMATERIAL COUPLED WITH HELMHOLTZ RESONATOR FOR ENHANCED ACOUSTIC PIEZOELECTRIC ENERGY HARVESTING

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ABSTRACT

To achieve high-performance acoustic piezoelectric energy harvesting at lower frequencies, this study proposes a metamaterial and Helmholtz resonator coupled structure. The metamaterial incorporates periodically arranged composite resonant pillars within a perforated thin plate. By designing a point defect in the metamaterial, vibration energy can be intentionally confined to the defect location under the defect band frequency. This design results in a more substantial energy localization for the coupled structure, leveraging the characteristic of amplified acoustic pressure in the Helmholtz resonator. Initially, the mathematical model for calculating the first resonant band gap is established. The band gap and corresponding defect band frequency are then validated by comparing finite element simulation with experimental results. Subsequently, numerical simulations are conducted to investigate the influences of hole size and coupled structure on acoustic piezoelectric harvesting energy. The results demonstrate a significant improvement in vibro-acoustic localization and piezoelectric conversion efficiency with an increase in the hole size of the perforated metamaterial plate. Furthermore, the synergistic effect of local resonance and acoustic pressure amplification generated by the coupled structure further enhances the performance of acoustic piezoelectric energy harvesting. At an acoustic incident amplitude of 2Pa and a defect band frequency of 1068.5Hz, the coupled structure attains the maximum output voltage and power of 5.94V and 39.10μW, respectively. These values are 2.65 times and 2.80 times higher than those of the uncoupled metamaterial structure. This study offers guidance for designing piezoelectric energy harvester applications in self-powered sensors and small electrical devices.

Modeling and simulation of coupled processes in geological media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FINITE ELEMENT-FINITE VOLUME COUPLED ASYMPTOTIC TIP ENRICHMENT FOR HYDRAULIC FRACTURE PROPAGATION

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ABSTRACT

Numerical strategies suitable for field-scale fluid-driven fracture simulations have significance in advancing the scientific understanding of natural phenomena in geoscience and disrupting the status quo of geological techniques. The accuracy and robustness of numerical strategies largely hinge on the appropriateness of fracture propagation criteria in different regimes and the capability to locate the fracture front position in discretized computational domains. We address the above topics in the context of a fully coupled finite element-finite volume computational framework. Based on the fracture tip asymptotic solutions, we solve the Eikonal equation using the fast marching method to calculate the signed distances at element nodes. The signed distance field is used as the fracture propagation criterion, where element nodes are split when the calculated distances change signs. This feature enables us to overcome the limitations associated with the conventional stress intensity factor-based approach in the viscosity-dominated propagation regime. From the signed distance field, we can also locate the fracture tip in partially opened elements, providing accurate fluid volume and transmissibility estimations to enforce the fluid mass conservation. This feature overcomes the numerical difficulties encountered in the fracture element initialization during a propagation time step, therefore facilitating the convergence of the tightly coupled finite element-finite volume solver.

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Modeling friction and wear
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APPLICATIONS OF THE FAST FOURIER TRANSFORMS TECHNIQUE FOR CONTACT ANALYSIS OF HETEROGENEOUS MATERIALS

Kuanyu Liu[1], Zhizhen Jiang[1], Hengxu Song[2], Pu Li[3], Feodor Borodich[1] and Xiaoqing Jin[1]*

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ABSTRACT

Contact problems are widespread in engineering applications, posing significant challenges due to the intricate interactions associated with diverse impurities[1, 2]. The complexities arise from the diversity in shapes and material properties of the inhomogeneities, contributing to the computational intensity associated with the discretization of numerous elements[3]. This necessitates innovative solutions to address the intricacies of these problems and improve computational efficiency. In response to these challenges, this paper introduces an innovative solution for solving the contact problems, leveraging the Fast Fourier Transform (FFT) algorithm.

The present approach not only addresses the complexities introduced by the diverse impurities but also capitalizes on the FFT algorithm's efficiency in handling the associated contact problems. By deriving the analytical solutions for stress in a semi-infinite medium, the work presents a structured methodology[1] that significantly enhances computational efficiency. The present approach not only streamlines intricate calculations but also mitigates the computational load, making it an attractive alternative for engineering analyses[2].

Furthermore, the proposed method's versatility is demonstrated through its application across different inclusion shapes and materials. The FFT-based algorithm proves to be a powerful tool in handling the diversity of contact problems, showcasing its potential to revolutionize computational methodologies in engineering applications[2, 3].

In essence, the utilization of FFT principles in contact problems not only enhances accuracy and computational efficiency but also offers a versatile and powerful solution. This approach represents a significant advancement in addressing the complexities of these problems, providing valuable insights for engineers and researchers in various fields.

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Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DISCRETE RITZ METHOD

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ABSTRACT

In the past century, the Ritz method could not be applied to complex geometric problems due to the complexity of constructing a global trial function to approximate structural behaviours and the difficulty of numerical integration in complex geometric domains. This fact has led to a large number of literatures examining the problems of two-dimensional (2D) and three-dimensional (3D) structures having regular geometries. Reddy[1] indicated that the Ritz method is a true "meshless" method because it uses a global trial function for solving the problem, thus eschewing the necessity for meshes or nodes in the solution process. However, engineering problems are significantly more complex with irregular geometries, preventing the Ritz method from being applied, despite the fact that it is "meshless", efficient, and accurate.

To resolve this problem, this study presents a novel numerical method, discrete Ritz method (DRM), for the static, stability and vibration analysis of 2D and 3D structures with arbitrary geometries[2-3].

The problem is formulated in a standard geometric domain (rectangle for 2D and cuboid for 3D problems), and arbitrarily shaped structures can be simulated by assigning cutouts within the standard geometric domain. Geometries of structures are characterized by using level set functions. By combining the extended interval integral, Gauss quadrature, variable stiffness characterization, the strain energy of the structure is modelled in the standard geometric domain, discretized using Gauss points, and is characterized by variable stiffness, which characterizes the material distribution and structure geometry simultaneously. In this manner, DRM transforms the problem into a discrete energy system which allows the geometric boundary of the structure to vary in the standard geometric domain. The orthogonal polynomials are used as the global admissible function to approximate structural behaviours. The deformation of arbitrarily shaped structures can be numerically simulated by setting the stiffness and thickness of Gauss points within the cutouts to zero. New formulations in DRM have resulted in completely standard energy functionals and computation procedures for arbitrarily shaped 2D/3D structures.

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Advanced techniques for transport phenomena in heterogenous porous media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FLOW AND TRANSFER LAWS IN SOLID FOAMS: REGIME TRANSITIONS AND STABILITY

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ABSTRACT

Optimal design of industrial systems such as reactors, columns or heat exchangers using foams as medium requires accurate prediction of transport properties, and remains a major concern today. Those porous media can be too complex for studying individual morphological features as we can not control individually each parameters (e.g., strut shape, pore elongation, etc). We have then chosen a simplified model consisting in a tri-periodic kelvin cell with varying strut size and cross-section.

The approach of numerical simulations at pore scale has become a popular criterion with the development of high performance computational power, used here to determine intrinsic macroscopic hydraulic properties on porous structures. The recent development of innovative scheme like Lattice Boltzmann (LBM) to overcome the classical drawback of commercial softwares (Finite Volume, Finite Element) in achieving high accuracy, shows the potential of kinetic based methods for producing efficient and accurate solvers. An alternative vector kinetic method is proposed to solve incompressible Navier–Stokes equations at pore scale and eventually determine permeability tensors of complex porous media. A moment based (vs discrete velocities), non-diffusive, explicit, parallel implementation was implemented and successfully used on several totally different complex geometries. Excellent results at low Reynolds number were obtained, the method is thus well suited for permeability tensors determination of complex heterogeneous media (e.g. sandstone, redwood samples).

We are also interested in the flow stability, studies being performed with homemade numerical tools, using Finite Element Methods. The first one uses a steady-state continuation algorithm, based on the Asymptotic Numerical Method (ANM) that enables to determine critical points along the continuation parameter path (here the pressure drop) where there is a steady-state bifurcation. The second tool studies the linear stability of the steady-state solution given by the ANM, and determine the critical pressure drop where the Hopf bifurcation (unsteady and periodic solutions) occurs. Using the above numerical methods, we have shown in recent results ([1]) the bifurcation diagram of a periodic Kelvin cell made up of triangular struts. Moreover, we have linked both (dynamical and state-state) bifurcation types to the macroscopic flow regimes (Darcy, transition, Forchheimer).

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INTERPOLATION BASED PARAMETRIC MODEL ORDER REDUCTION USING MODIFIED COMPONENT MODE SYNTHESIS

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ABSTRACT

Model Order Reduction (MOR) techniques are widely used in reducing the computational time associated with simulating high-dimensional models, enabling faster analysis and optimization processes [1,3]. Projection-based methods are generally used for MOR of dynamical systems. In these methods, the governing equations in the high dimensional space are projected onto a lower dimensional subspace using a transformation matrix which consists of projection bases. Component Mode Synthesis (CMS) is a very popular method frequently used for structural systems along with substructuring. The information loss of CMS is mainly associated with its part-static nature due to static condensation. We propose a Modified Component Mode Synthesis (MCMS) method based on the highly efficient method [2] that considers the dynamic nature of the model. The ease of computing the transformation matrix with the help of a recurrence formula makes the method more computationally efficient than iterative schemes. This paper presents an interpolation based parametric model order reduction (pMOR) with the application of MCMS along with substructuring. Heavy computational resources are required to investigate the parameter dependency of the entire system having multiple parameters. Therefore, the offline sampling is done at the substructural level to save computational time [3]. Each substructure is reduced using MCMS scheme. A congruence transformation matrix is also computed to retain the accuracy of the ROM while interpolation. In the on-line stage, the ROM is constructed by interpolating the already sampled ROMs at the subdomain level. Global assembly is done ensuring the compatibility of substructures. The interface degrees of freedom of the ROM are also reduced enabling the construction of two-level semi-parametrized ROM [3]. The accuracy and efficiency of the proposed method is demonstrated by computing the relative eigen-value errors and comparing the transient response of one dimensional and two dimensional structural systems at some random parameter within the sampling range.

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Industrial applications of IGA
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GENERALIZED PARAMETRIC MODELING AND ISOGEOMETRIC ANALYSIS OF STENTED MEDICAL DEVICES

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ABSTRACT

Stents are an essential therapeutic intervention approach to address various medical conditions and diseases across the entirety of the human anatomy, including the heart, vascular system, brain, lungs, and kidneys. Even with the maturity of many stent technologies, device designs across different physiological environments exhibit immense variability despite experiencing relatively similar mechanical conditions. Stent structures can be utilized for specific shunting or drug-eluting purposes. These stents are typically made from biocompatible materials such as stainless steel, cobalt-chromium alloys, or advanced polymers for bioresorbable variants. The technical complexities of stent design include various considerations. One such aspect is the interlocking pattern, which impacts each device’s stress distribution, manufacturing difficulty, and durability. Another critical factor is the strut thickness, which influences the stent’s radial strength and flexibility during the crimping and expansion processes. Additionally, the inter-strut angles are crucial for ensuring sufficient friction with the vessel walls while minimizing blood flow disturbance. This study develops parametric models for stents referencing real-world cases based on a novel, bio-inspired, unit-cell-based platform for a generalized stent model. Each "cell" shape is modified locally, and the height, width, and orientation are adjusted to generate a stacked unit-cell column that is revolved radially about a central axis to generate the full stent model. This method allows for straightforward localized modification, customized geometry extension in multiple directions, and more optimization choices. This model enables various developments in modeling stents using the proposed approach, including assessing multi-directional unit cell combinations, creating unit cell patterns with unique shapes, and exploring performance differences between open and closed cell structures. The proposed methods aim to enhance the versatility and effectiveness of stented devices through efficient computational modeling using isogeometric analysis. Future investigations will also integrate these modeling approaches with performance-based assessments to improve the function and long-term performance of stented devices.

A PSEUDO-DIFFERENTIAL SWEEPING METHOD FOR THE HELMHOLTZ EQUATION USING HIGH ORDER SPECTRAL ELEMENTS

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ABSTRACT

Ultrasound-guided medical procedures often experience complications when imaging heterogeneous tissue. Computer simulations of the ultrasound field offer a workable solution to this heterogeneity problem, but the computational methods required for these simulations tend to be either highly accurate and computationally slow or computationally quick and inaccurate. We propose a sweeping numerical method for solving the Helmholtz equation which is built from a truncated pseudo-differential expansion. We discretize this expansion using high order spectral element methods in space and an explicit time-stepping method in time. Numerical experiments examine the behavior of the proposed method in 1D and 2D under different numerical parameters. We demonstrate that the proposed sweeping method is not only accurate but increases in accuracy as the angular frequency increases.

ADAPTIVE AND SCALABLE DOMAIN DECOMPOSITION PRECONDITIONERS

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ABSTRACT

Recent advances in adaptive domain decomposition methods have made it possible to solve large systems of equations that where previously challenging for both algebraic multigrid (because of lack of robustness) and exact factorization (because of large FLOP count and memory cost). In this presentation, I will highlight some recent improvements and developments in PETSc, the Portable Extensible Toolkit for Scientific computations, and one of its preconditioner, PCHPDDM, a framework for defining efficient domain-decomposition based preconditioners. Numerical results for solving large coupled systems of various types (such as indefinite or nonsymmetric) will be showcased.

Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MACHINE LEARNING APPROACH TO FAST STATISTICAL MICROSTRUCTURE PREDICTIONS IN LASER POWDER BED FUSION WITH ARBITRARY PROCESS PARAMETERS

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ABSTRACT

The laser powder bed fusion (LPBF) additive manufacturing process produces complex microstructures, which have been shown to vary with process parameters and print geometry. Because the process is slow and multiscale, it is not feasible to tune the process parameters for every new part geometry via experimentation or traditional computational modeling. A previously introduced fast machine learning based microstructure model can reliably predict statistics about LPBF-produced microstructures orders of magnitude faster than equivalent simulations. This work analyzes the effectiveness of this fast machine learning based microstructure model by assessing the model's predictive power and the minimum viable training dataset. Efficient strategies for making part-scale predictions are explored.

Constitutive modeling of complex materials with machine learning and artificial intelligence
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ACCELERATING MULTISCALE SIMULATION WITH MACHINE LEARNING

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ABSTRACT

Multiscale simulation is needed in cases where a single representative constitutive model cannot be constructed for the material of interest due to inherent or designed inhomogeneities in the microstructure. Classical multiscale methods rely on subgrid/mesh solves for microstructual samples which are coupled by an equilibrium equation for the full structure. Machine learning via convolution neural networks enable the accurate and efficient encoding of these microstructural response functions. This talk will describe the particular architecture and demonstrate the efficacy of neural networks designed to model the response of microstructural samples. In addition, the models are incorporated in a large-scale simulator that enables material uncertainty quantification and design under uncertainty. Representative boundary value problems will demonstrate the utility of the approach and its correspondence with direct numerical simulation of large-scale structures with microstructural details.

Fluid-structure interaction in interface and moving boundary problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VARIATIONAL HYDROACOUSTIC FORMULATION FOR MOVING BOUNDARY PROBLEMS

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ABSTRACT

Motivated by the stealth-like low acoustic signature in the flapping motion encountered in fishes, the current study focuses on developing a computational framework for modeling hydroacoustics in moving boundary problems. Several acoustic formulations based on integral methods (FW-H and Curle's method) and perturbation equations (Linearized Euler Equations, Perturbed Compressible Equations [1] , Acoustic Perturbed Equations [2]) have been proposed in the literature. However, either these methods are inaccurate or computationally expensive due to the increase in variables in the form of perturbed quantities. Hybrid techniques decompose the flow variables into incompressible and acoustic components so that a solution from an incompressible solver can be coupled with an acoustic solver. Moreover, implementing the acoustic solver is complicated, and higher-order methods are generally used for discretization.

For hydrodynamic problems, the flow can be assumed to be at low Mach number, and temperature variations can be neglected. This simplifies the governing equations such that pseudo-compressibility can be incorporated into mass and momentum conservation equations [3] . These equations circumvent the need for perturbed equations and lead to fewer unknowns for the problem. The current study implements the pseudo-compressible Navier-Stokes equations in the moving mesh arbitrary Lagrangian-Eulerian framework for moving boundary problems. The equations are discretized using stabilized finite element methods with equal interpolation for the flow variables. Benchmarks test of flow across a stationary cylinder at Reynolds number of 200 and Mach number of 0.3 is conducted to verify the acoustic propagation. The study then demonstrates the ability of the solver to predict the acoustic signature of a rigid passively flapping foil at a Reynolds number of 1100.

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Computational particle-based solvers for multiphysics & multiscale simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE EFFECT OF BOUNDARY CONDITION FORMULATIONS ON BULK DEPOSITION PROPERTIES FOR 3D CONCRETE PRINTING USING THE MATERIAL POINT METHOD

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ABSTRACT

Additive manufacturing (AM) is fast becoming a disruptive technology in the manufacturing space. AM promises to provide engineers and designers with increased flexibility in their designs, allowing for the manufacturing of objects that are impossible with conventional manufacturing techniques. While most AM technologies target small-scale plastic or metal parts, 3D concrete or earth-based material printing is a niche AM technology that aims to print large-scale 3D concrete structures by following a similar process to the classic extruded material method (EMM) using custom concrete compositions designed to control the material properties and setting behaviour.

Tuning of the printing process is typically required to produce high-quality prints with both the desired macroscopic mechanical properties and the required final shape. Simulations can reduce the number of iterations necessary for tuning, which is especially important for concrete printing due to the time and repreparation cost of the process. The EMM process naturally benefits from a Lagrangian description, especially when considering the multiphysics nature of this process.

The material point method (MPM) [1] is a numerical scheme that discretises a system as Lagrangian material points. Mapping material point properties to an underlying Eulerian grid enables resolving differential operators. The grid state is updated and mapped back to the particles. These two system representations naturally enable two domains to develop and enforce boundary conditions: grid- [2] and particle-level [3] boundary schemes.

For 3D concrete printing, the formulation and implementation of boundary conditions can affect the final predicted footprint and shape. However, the implications of particle-based or grid-based boundary condition enforcement require further investigation. This work addresses this by presenting a multiphysics MPM formulation for 3D concrete printing that allows for comparisons between different particle-based and grid-based boundary condition schemes. This study simulates, verifies, and conducts a sensitivity study of process parameters on a single concrete layer's deposition.

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ON MODELLING THE FREQUENCY DEPENDENCE OF UNFILLED AND FILLED ELASTOMER BLENDS

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ABSTRACT

Elastomer blends are of high interest for tailoring materials with specific mechanical behaviour. However, while for the pure components the experimental characterization of the temperature dependent viscoelastic properties is usually well feasible, doing this for the blends is often difficult or impossible.
One reason is that the blend components often have different glass transition temperatures which makes the resulting behaviour quite complex.
In most cases when blending elastomers, heterogeneous morphologies are formed consisting of different regions with (nearly) pure components and finite interphases in between. In addition to the pure phases, especially these interphases influence the resulting viscoelastic properties significantly. For such cases, material modelling and numerical simulations can help to better understand the interactions between phases and interphases and to forecast the resulting viscoelastic properties.
In this contribution we model and simulate an RVE of a binary blend consisting of natural rubber (NR) and styrene butadiene rubber (SBR). The modelling and the simulations are performed in the small strain regime, using linear viscoelasticity. A phase field variable is used to describe the blend morphology within the simulation. The blend morphology is based on microscopic images and the dependency on the field variable is derived from an energy formulation allowing sharp and diffuse interphases between the NR and SBR phases. Both, sharp and different diffuse interphases are numerically investigated and their influences on the mechanical behaviour are compared to elaborate experiments.

Multi-scale and machine learning-based modeling methods for optimization and design of composites
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

UV-IRRADIATION EFFECT ON ATOMIC OXYGEN RESISTANCE OF POLYMER MATRIX IN LOW EARTH ORBIT ENVIRONMENT

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ABSTRACT

In the low earth orbit (LEO), polymer matrices in spacecraft structure experience harsh environments including atomic oxygen (AO) collision, ultraviolet (UV) irradiation, thermal cycle, high vacuum, etc. Especially, highly reactive AOs lead polymer matrices oxidized and eroded at the surface, resulting in degradation of mechanical properties of structures and critical failure of electrical systems. Therefore, several researches were conducted improve atomic oxygen resistance of the polyimide (Kapton) and epoxy, which are thermal insulation coating material and structure material in LEO satellites, respectively. However, not only in-flight experiments but in-ground experimental simulations are also costs high economic and temporal resources in describing environments in LEO (high-UV, high-vacuum, AO, extreme temperature cycles, etc.) and long duration of the experiments. Thus, molecular dynamics simulations with reactive force fields which are able to describe active formation of chemical bonds during oxidation by AO collisions, had been conducted. Evaluation of AO resistance through reactive MD simulations of Kapton nanocomposites, epoxy, silicon carbide, etc., were reported for last decades. To simulate polymer degradation by UV-irradiation, density functional theory (DFT) studies were reported to predict dissociation of crosslinking bonds in epoxy. The synergetic effect of UV and AO erosion were consistently investigated by experiments that up to 400% increase in erosion rate by AO were observed when 172nm vacuum UV were exposed on polyimide films. However, such synergetic effects between UV and AO collision had not been reported through molecular simulations. Therefore, in this study, acceleration of the AO erosion by chemical bond degradation in polymer matrix through UV irradiation will be discussed through multi-scale scheme combining DFT and reactive MD simulations.

SPACE-TIME MODELING OF MATERIALS WITH DISSIPATIVE MICROSTRUCTURE EVOLUTION VIA STATIONARY PRINCIPLES

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ABSTRACT

Material modeling is a core task in the research of mechanics of materials. Starting from the experimentally observed phenomena, appropriate variables have to be defined which enable us to describe the material behavior. These variables are usually referred to as internal variables and complete the set of thermodynamic state variables. There exist different methods to derive equations which describe the evolution of the internal variables and thus, the evolution of microstructure. In the end, the (numerical) solution of the resultant coupled system of algebraic-differential equations, often with inequality constraints, paves the way for in-silico experiments and, consequently, improve our understanding of the physical processes in material behavior and offers the possibility to design construction parts with tailored properties.

Usually, the system of equations is the starting point for a space-time description: this strong form is then multiplied with appropriate test functions and integrated over space and time to receive the weak form. Appropriate discretization schemes can be invoked for numerical solution. Here, it might be unclear which function space is needed for the test functions in the respective equations.

In this talk, we present a different approach for holistic space-time material modeling: by careful analysis of Hamilton’s principle, which contains as special case the principle of least action, the space-time formulation of arbitrary material models can be obtained from a stationarity principle. This, for instance, directly solves the issue of appropriate function spaces. We present that Hamilton’s principle is not restricted to elastic problems. In contrast, it can be used for materials with ordinary and partial differential equations or inequalities as evolution equations. We furthermore showcase that also Navier-Stokes equations directly follow from this principle which then enables us to make use of the concept of internal variables also for modeling of non-Newtonian fluids. Exemplarily, we demonstrate this for fluids with fading viscosity which models the bidirectional laminar/turbulent transition.

Advances in computational biomechanics and mechanobiology
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GENERALIZED STRUCTURE TENSOR-BASED SWITCHLESS CONSTITUTIVE RELATIONS FOR ARTERIAL TISSUES

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ABSTRACT

The collagen fibers which provide mechanical reinforcement to the arterial wall cannot sustain compressive loads. The existing Generalized Structure-Tensor (GST) based formulations emulate this through a tension-compression switch criterion based on the fiber stretch. This approach, however, has the following drawbacks:
1. discontinuous stresses at the switch point,
2. inconsistent predictions of the fiber stretch due to the conditional constitutive relations, i.e., the fibers predicted to be in compression according to the anisotropic terms can be in tension after the switch is employed, and
3. identical responses in longitudinal and transverse shear of unidirectional fibers, contrary to experimental observations.

To address these concerns, we introduce a matched invariant based on the Seth-Hill strain measure that auto-annihilates the contribution from fibers in pure compression. This leads to a unitary & switchless constitutive relation. The matched invariant inherently contains the I5 invariant and, consequently, the different shear modes yield distinct responses. The definition of the matched invariant is generalized for distributed fibers using the GST approach.

A vanishing matched invariant-based GOH (Gasser-Ogden-Holzapfel) constitutive relation with the same number of material parameters is obtained as a particular case corresponding to the Green-Lagrange strain. The constitutive relation with the general Seth-Hill strain resembles an anisotropic Ogden-like relation that can better control the relative magnitude of normal and shear stresses. For deformations devoid of shear, the proposed relations exclude the compressed fibers in a manner similar to that of the angular integration-based model proposed by Li et. al [1]. As evidenced by extensive fitting to planar biaxial and uniaxial data for various arterial tissues, the resulting unitary constitutive relations have significantly improved descriptive and predictive capabilities. The proposed switchless constitutive relation solves the discussed issues with little added complexity. This formulation is equivalent to using a modified and deformation-dependent structure tensor instead of the conventional GST, thereby eliminating the major hurdles associated with the use of a switch criterion.

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Machine learning for large scale models in physics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ELASTICITY BASED MESH DEFORMATION TECHNIQUE AND APPLICATION TO REDUCED ORDER MODELLING

Abbas Kabalan[*1], Fabien Casenave[2], Felipe Bordeu[2], Virginie Ehrlacher[3] and Alexandre Ern[3]*

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ABSTRACT

In this work, we develop an algorithm to build a mapping between two geometries based on elastic deformation. While many elasticity-based approaches exist in the literature, the proposed method can be used for non-parametric geometries. The aim of this tool is its use in some surrogate modeling techniques or projection based model order reduction, where we are interested in accelerating the computation of solutions for complex parametric physical models with geometric variabilities. Many of these methods require each new domain to be mapped to a reference domain where the prediction/calculation can be performed. However, very often in practice, we don't have access to a domain parametrization, and only a mesh for a new geometry is available. In this case, our method can be used to construct such a mapping.

First, given a family of target domains, we start by applying the method to build a mapping between a common reference domain and each target domain. The mapping takes into account geometric features such as labeled lines and points, like the position of application of boundary conditions, so that each label in the reference geometry is aligned with its correspondence in each target geometry. Since we are interested in surrogate modeling, and to achieve online efficiency, all these calculations are performed during the offline phase. Then, for the online phase, we propose a reduction technique to efficiently build the mapping for a new unseen geometry, making our method effective for online use for surrogate modeling or projection-based model order reduction.

Contact and interface mechanics: Modeling and computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN ARBITRARY ORDER CONTACT FORMULATION USING LAGRANGE MULTIPLIERS FROM RAVIART-THOMAS SPACE

Lukasz Kaczmarczyk[*1], Chirs Pearce[1] and Adnrei Shvarts[1]*

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ABSTRACT

We will present an approach for the analysis of contact in the context of elastic and elastoplastic materials. In the case of elastoplastic materials, we will use the multifield plasticity formulation [1]. The advantages of the presented finite element technology will be shown as examples of deformation of meta-materials, incremental cold forming of metals, and deformation of the rough multi-scale surface of Triboelectric generators. However, the focus of the talk will be dedicated to the core problem, stability of contact formulation of Lagrange multipliers, and solution schemes and efficiency for saddle point problems.

One established approach to enforce contact conditions is via the Lagrange Multipliers (LM) field, which is robust and implementation-independent from chosen material models. A consistent approximation of the LM field for h-refinement approaches has been developed and investigated [2, 3, 4]. However, p-refinement approaches are gaining popularity with the standardisation of hierarchical basis functions and a proper choice of basis functions to meet the needs of different functional spaces. For the case of contact problems, the space H^{−1/2}(Γ_c) is the LMs for contact when displacements are sought in the H^{1/2}(Γ_c) space. In the present work, a so-called dual approach for modelling contact of a deformable solid coming into contact with a rigid surface is proposed and is the first step towards a mortar contact formulation. The discrete functional space for LMs, H{−1/2}(Γc) defined on contact surfaces, Γ_c, emerges from the trace of Raviart-Thomas space, RT ⊂ H(div; Ω), defined in the deformable discretised body domain Ω^h. This enables us to evaluate some terms present in contact formulation both on the boundary and within the volume via the Gauss theorem, providing stability to the discrete solution.

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IMPROVED NEURAL OPERATOR WITH GRAPH CONVOLUTIONAL NETWORKS AS A REDUCED ORDER MODEL

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ABSTRACT

A Reduced Order Model (ROM) provides a viable alternative to Full Order Models (FOM) for large-scale optimization or real-time control tasks. However, ROMs, particularly Machine Learning (ML) -based, face challenges in large-scale industrial settings due to a scalability. To elaborate, each degree of freedom (DOF) corresponding to the discretization of the domain serves as input features. This leads to a significant increase in computational resource requirements as the problem domain expands, a common scenario in large industrial reservoir models, rendering the training process impractical.

To address this, we have developed the Improved Neural Operator (INO), an advanced neural operator that effectively divides the computational area into smaller segments for each training step [1]. This approach involves sampling our computational domain at each forward pass, leading to much smaller training sets compared to using the entire domain. The INO framework can adapt to training with various DOFs, even with limited portions of the computational domain. For instance, in the Illinois Basin – Decatur Project, INO achieved an average relative error below 1% for pressure predictions on the test set, using just 90 training samples over four years, a count considerably lower than standard deep-learning datasets.

Despite these advancements, INO encounters challenges in gaining a comprehensive global understanding due to its approach of subsampling. While INO's training speed is impressive, it assumes that the state of a Partial Differential Equation (PDE) is determined only by localized conditions. This assumption is limited in geological contexts that require understanding solution states over a broader area. For example, the INO model's random subsampling method does not provide a full view of a heterogeneous permeability field, exposing the model to different segments of the domain rather than the whole, simultaneously. This results in a partial understanding of the permeability field's values and connections, potentially leading to inaccuracies in predictions.

To enhance INO's capabilities, we propose integrating Graph Convolutional Networks (GCNs). GCNs utilize graph structures, like those in heterogeneous permeability fields, to extend the model's global perspective while maintaining localized training samples. This integration is designed to boost INO's overall performance and realism, offering a more accurate depiction of the intricate interactions within the permeability field.

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Machine learning for design tasks and inverse problems
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UNDERSTANDING AGENT ACTIONS UTILIZING ACTOR-CRITIC ALGORITHM IN DEEP REINFORCEMENT LEARNING

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ABSTRACT

Reinforcement learning has been applied to a broad range of problems and has achieved remarkable results, especially when combined with deep learning. However, such high-performance AI often leads to complex black-box models. That is the reason why explainable AI, which aims to make the predictive process of AI understandable to humans, is gaining attention.
In this research, we propose a method to visualize the rationale behind the actions of reinforcement learning agents by applying the Actor-Critic algorithm. Specifically, this involves estimating the rewards for the actor's actions based on the value inferred by the Critic, which evaluates actor's actions. Additionally, we developed a method for extending this approach to multi-objective optimization problems by creating a critic for each objective function. Sub-rewards, which were traditionally aggregated before being passed to the critic, are now explicitly passed to the critic. This allows the critic to learn the value function for each sub-reward and calculate sub-reward estimations.
To verify the usefulness of this method, we applied it to the pendulum problem, a benchmark problem in multi-objective optimization. Furthermore, we applied it to multi-objective optimization of turbine blades as an engineering application. For evaluation, we used the explanations derived from traditional reinforcement learning metrics such as loss and reward transitions and SHAP, a representative method of Explainable AI, as comparison targets to confirm an improvement in explainability. As a result, explanations that could not be provided by traditional methods were achieved with the proposed method. Remarkably, some of the results make it possible to definitively identify agent actions as mistakes, which could not be conclusively determined by means of traditional methods. Moreover, the results from this proposed method were often interpretable not only by developers and designers but also by non-professional.

FLOW-BASED QUANTIFICATION OF THE EPISTEMIC UNCERTAINTY OF SIMULATION PREDICTIONS

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ABSTRACT

We demonstrate how normalizing flows (NFs), a class of generative deep learning problems, can be applied to simulation predictions to quantify epistemic uncertainties. NFs use invertible deep learning architectures to solve the change of variables equation for probability densities. One density is prescribed (a.k.a. the “base” density, usually a high dimensional isotropic Gaussian) while the other density of the “target” data is learned. Crucially, the probability density of the target data is explicitly and tractably quantified. If the target data is, for example, a set of proton radiographs predicted by a simulation then the NF will “learn” an arbitrarily complex high dimensional target density in which the predicted radiographs are maximum likelihood. Then, if proton radiographs from an experiment are passed through the NF, the NF will compute the likelihood of the experiment radiographs within the density of the simulated radiographs. In other words, NFs quantify epistemic uncertainty by quantifying of the likelihood of any new sample within the learned target density. Provided sufficient numbers of training samples, this unsupervised method can be applied to high dimensional data.

SciML in the real world
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GEOMETRIC OPERATORS & GENERIC PARAMETRIC MODELING FOR AI-BASED SHAPE OPTIMIZATION IN MARITIME ENGINEERING

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ABSTRACT

Despite the recent spectacular successes of Artificial Intelligence (AI), the degree of its acceptance by the Engineering Design communities remains limited. This is especially true for Shipping, a conservative sector partially due to the long life-cycle of ships (25-30 years). In fact, the dominant design practice in Maritime Engineering, based on Parametric Modelers, which generate thin Design Spaces around a baseline design with costly, e.g., CFD and FEM simulations, has a limited capability for novelty.

Our work aims to strengthen AI's role in Engineering Design by deriving novel physics-informed and low-cost geometric functionals, acting as: (i) stabilisers versus the criteria of geometric-validity and shape-richness, and (ii) shape-optimisation accelerators in the Design Spaces and their latent subspaces involved. Our investigation covers so far a variety of application areas, such as flows around ships, propellers and hydrofoils, with very encouraging results, see, e.g., [1] and [3].

Furthermore, our recent research activities contributed towards establishing a novel paradigm in the area of Ship Design via a Generic GAN-based Parametric Modeler [2], which increases dramatically the capacity of generating novel shapes, while securing geometric-validity along with high-quality and low computational cost of the adopted shape encoding.

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Multiscale methods for advanced manufactured materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ACCELERATED DEVELOPMENT OF MATERIALS USING HIGH-THROUGHPUT STRATEGIES AND AI/ML

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ABSTRACT

The dramatic acceleration of the materials innovation cycles is contingent on the development and implementation of high throughput strategies in both experimentation and physics-based simulations, and their seamless integration using the emergent AI/ML (artificial intelligence/machine learning) toolsets. This talk presents recent advances made in the presenter's research group, including: (i) a novel information gain-driven Bayesian ML framework that identifies the next best step in materials innovation (i.e., the next experiment and/or physics-based simulation to be performed) that maximizes the expected information gain towards a specified target (e.g., optimized combination of material properties, refinement of a material constitutive response), (ii) computationally efficient versatile material structure analyses and statistical quantification tools, (iii) formulation of reduced-order process-structure-property models that enable comprehensive inverse solutions needed in materials design (e.g., identifying specific compositions and/or process histories that will produce a desired combination of material properties), and (iv) high throughput experimental protocols for multi-resolution (spatial resolutions in the range of 50 nm to 500 microns) mechanical characterization of heterogeneous materials in small volumes (e.g., individual constituents in composite material samples, thin coatings or layers in a multilayered sample). These recent advances will be illustrated with case studies.

Constitutive modeling of complex materials with machine learning and artificial intelligence
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATION OF PHYSICS-AUGMENTED NEURAL NETWORKS TO MULTISCALE PROBLEMS

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ABSTRACT

Due to the recent development of machine learning, constitutive models based on neural networks are becoming increasingly popular. Thereby, a promising field of application is the usage of such models for the acceleration of multiscale simulations [1].

Herein, we present an approach based on physics-augmented neural networks (PANNs) [2,3] that are applied as macroscopic surrogate models. PANNs are designed to fulfill as many conditions as possible from constitutive modeling by construction and are very flexible at the same time. Our approach allows the efficient simulation of materials with complex underlying microstructures which reveal an overall anisotropic and nonlinear behavior on the macroscale. Thereby, we restrict ourselves to finite strain hyperelasticity problems in the first part of the talk. By using a set of problem-specific invariants as the input of the PANN and the Helmholtz free energy density as the output, several physical principles are fulfilled a priori [2,3]. The invariants are formed from structure tensors and the right Cauchy Green deformation tensor. Necessary data for the training of the PANN surrogate model are collected via computational homogenization of representative volume elements (RVEs). Besides the network parameters, the structure tensors are automatically calibrated during training so that the underlying anisotropy of the RVE is reproduced in the best possible way. The developed approach is exemplarily applied to several descriptive examples. Finally, an extension of the approach to magneto-hyperelasticity is shown [3].

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PHASE-FIELD MODELLING OF DUCTILE FATIGUE FRACTURE

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ABSTRACT

Phase-field modelling of fatigue fracture has been approached by many different models in recent years. Yet due to the high number of load cycles involved, computational time remains one of the main challenges, especially for fracture in ductile materials such as metals.

In this contribution, we revisit our efficient phase-field model for fatigue fracture [1] with a simplified consideration of cyclic plasticity. We combined the phase-field method for brittle fracture with the Local Strain Approach [2], a traditional fatigue concept from structural durability. It involves assumptions for the stress-strain behaviour including local plasticity and the damaging effect of load cycles, based on experimental material data.

Now, we improve the model by refining both the approximation of the stress-strain behaviour and the evaluation of the damaging effect of the load cycles with a new damage parameter. In a second step, we introduce a comprehensive phase-field model with elastic-plastic material law [3]. This we use to evaluate the two efficient models with the simplified integration of plasticity. The range of application of the three models is discussed, compromising between accuracy and computational time.

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THE MICROLAYER MODEL – A NOVEL APPROACH TO DESCRIBE MATERIALS WITH RIGID PARTICLES EMBEDDED IN A MATRIX

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ABSTRACT

Concrete is one widely utilized material. Due to its heterogeneous mesostructure, it exhibits specific material characteristics. Firstly, concrete can withstand larger loads in compression than in tensile regime. Secondly, under multiaxial loadings, concrete shows a significant influence of the secondary loading directions. Significant differences in the directional stiffness along the different loaded directions are typical for concrete. To overcome the limitations with respect to load bearing characteristics under tension, reinforcements are utilized.

In computational mechanics, concrete is often modelled by the so-called microplane material model, which is based upon linking the behavior of a material point with a representative volume element. In the microplane framework, unit spheres are chosen for representing the material behavior of concrete. Also, this model is not based upon the Principle of Multiscale Virtual Power according to the authors knowledge. The utilization of the aforementioned principle results in better agreement with reality.

In the contribution at hand, a new approach to model concrete, the microlayer model, is detailed and applied in numerical simulations. The formulation can be generalized to all materials, which consist of rigid particles embedded in a deformable matrix. One main advantage of this modelling strategy is, that anisotropy, which is induced by loading, can be captured in a closer alignment with experimental data. In the microplane material model, the directional stiffness is shown to only exhibit small differences, while for the microlayer material formulation significant differences can be observed. Another class of models, which rely on the concept of homogenization, are FE^2 formulations. In the microlayer model, the smaller scale is solved analytically, which results in significantly reduced computational effort.

The capabilities of the microlayer material formulation are shown for different numerical examples. Firstly, numerical simulations are conducted to compare the behavior of the microplane and microlayer material model. Subsequently, experiments on concrete are simulated to validate the microlayer model.

16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Minisymposium in honor of Prof. Yannis Kallinderis's 60th birthday: Progress of Unstructured grid based CFD, hybrid mesh generation and adaptation, and parallel supercomputing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DISCRETIZATION ERROR ESTIMATION FOR FLOW SIMULATIONS USING GENERAL HYBRID GRIDS

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ABSTRACT

The discretization error is a primary component of the numerical error in flow simulations. Use of general hybrid meshes is of importance due to the complexity of both the geometry and the field of modern computational fluid dynamics applications. The meshes can consist of a mix of hexahedra, prisms and tetrahedra with pyramids being transitional elements. The different elements are arranged in local areas of different grid density and directionality according to the dominant flow feature there. The discretization error arises not only from the local density of the mesh, but also from its "distortions", namely the local size variation (stretching), the shape of the individual elements (shear, skewness, twist), as well as the local change in their type (grid interfaces).

Two distinct approaches have been followed in order to estimate and control the discretization error: the a priori methods are employed during grid generation and its assessment (e.g. [1]) and the a posteriori ones monitor the simulated flow field and guide grid improvement (adaptation) (e.g. [2]).

The a priori approach utilizes a second order finite volume discretization. It derives expressions of the truncation error for the most commonly encountered "distortions" of the mesh and works with the terms that multiply the solution derivatives (grid metrics or error coefficients). The magnitude of those terms is used to guide grid generation and post-processing of the initially created grid.

The a posteriori error estimation monitors approximations of the magnitude of the flow gradients ("sensors"). Those are then applied to guide adaptation of the grid to the simulated flow field. This typically includes local divisions of the elements or entire zones, grid point / element redistribution or local change in the order of discretization.

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Physical models and reduced order models augmentation with data for physics-informed machine learning in real-world applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NEW LOSS FUNCTION FOR EFFICIENT LEARNING OF PARAMETRIC PHYSICS INFORMED NEURAL NETWORKS

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ABSTRACT

Physics informed neural networks (PINNs) has emerged as a surrogate modeling method garnering considerable attention. It incorporates the governing equations of physical phenomena into the loss function, enabling efficient and highly accurate learning with minimal observation data. Consequently, PINNs has been applied in various fields where there is a lack of observation data and real-time predictions are essential, including aerospace, mechanical engineering, architecture, civil engineering, and the medical field. In design problems, parametric PINNs is expected to facilitate rapid and precise uncertainty quantification and optimization, with growing research interest in this area.

In this study, we focus on the learning of parametric PINNs with limited observation data along the parameter axis, aiming to enhance efficiency. We propose introducing a new loss function term, the "parameter gradient loss," which derives from the parameter derivative of the governing equation. To assess the impact of this new term, we explored how the weight during learning and the number of observation data along the parameter axis affect performance using a simple static one-dimensional Euler beam problem as a case study.

Our results indicate that the proposed method can reduce prediction error in the interpolation range, even under challenging learning conditions, such as sparse observation points along the parameter axis and the absence of evaluation points of the governing equation between observation points, compared to traditional approaches. We observed that increasing the learning weight reduced the prediction error of the interpolation range. However, the error increased beyond a certain weight threshold. Conversely, the effectiveness of the proposed method was limited with a relatively higher number of observation points along the parameter axis than in our other computations or when evaluation points of the governing equation were placed between observation points.

This study introduces a novel loss function for efficient learning in parameteric PINNs, demonstrating its potential even with sparse observation data in the parameter direction. This approach is anticipated to lessen the need for extensive numerical analyses and experiments for each parameter set before learning in parametric PINNs, offering significant benefits in practical computational settings.

Data-driven modeling and design of materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A PHYSICS- AND DATA-DRIVEN FRAMEWORK FOR HIGH THROUGHPUT DEVELOPMENT OF HIGH ENTROPY ALLOYS

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ABSTRACT

High Entropy Alloys (HEAs) have shown potential to improve on the performance of legacy materials, thus characterizing the relationships between the composition, material properties, and microstructure of HEAs is of great interest. However, predicting these characteristics presents significant challenges due to the complex, multi-component nature of HEAs and the resulting large design space. To address this challenge, a multi-physics simulation framework and data-driven surrogate modeling approach are implemented, to provide a method to rapidly assess how changes in HEA composition will lead to changes in material properties and microstructure. The physics-based framework sequentially couples CALPHAD for material properties, CFD for thermal conditions during solidification, and Cellular Automata for microstructure. A data-driven surrogate model, which can reconstruct microstructure statistics from the thermal conditions, is trained via a reduced-dimensional form of the microstructure output of the physics-based framework. Dimensionality reduction is achieved in two steps. First, Angularly Resolved Chord Length Distributions (ARCLDs) are extracted from microstructures by sampling the distance between grain boundaries at various angles. ARCLDs provide a thorough statistical characterization of microstructure morphology and are a robust representation of microstructure as a result. Second, the ARCLDs are reduced via Principal Component Analysis (PCA), resulting in identification of the significant modes of each Chord Length Distribution. The coefficients of these modes are the final reduced form of the microstructure and are the output for which the surrogate model is trained. The coefficients which are output from the surrogate model are used with the significant PCA modes to reconstruct the ARCLDs of the microstructure, providing insight into how thermal conditions will affect microstructure characteristics without having to run a slow microstructure simulation. This surrogate modeling approach provides a significant speedup to characterizing the relationships between HEA composition, thermal conditions, and the final microstructure. This combination of physics-based and data-driven approaches with a reduced-dimensional representation of microstructure can significantly speed up the development of HEAs, increasing their adoption rate in practical applications. Additionally, the ability of the present surrogate model to reconstruct a statistical representation of the microstructure lays the groundwork for future endeavors to reconstruct the microstructure itself.

Imaging-based methods in computational medicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A FINITE ELEMENT INFORMED NEURAL NETWORK (FINN) FOR ELASTOGRAPHY

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ABSTRACT

Elastography is an imaging technique utilized for extracting tissue elastic modulus from various imaging modalities like ultrasound, MRI, and video cameras. While in practice, the application of elastography has encountered challenges in achieving accurate quantitative analysis within computational mechanics. These challenges stem from human factors, ad hoc assumptions, and image quality issues, limiting broader applications. Current data-driven models in elastography heavily rely on large datasets, leading to statistical sensitivity. In response to these limitations, we propose an innovative approach that integrates physics-based models using the Finite Element Method (FEM) with Deep Neural Networks (DNN). We term the approach Finite Element Informed Neural Network (FINN). Our method incorporates mechanistic understanding of physics principles into deep learning, enabling precise capture of ultrasound deformation without the need for extensive training datasets. The algorithm demonstrates robustness across diverse scenarios, displaying an error margin of less than 5% compared to ideal conditions. Validation of the algorithm against ultrasound testing on tissue-mimicking phantoms further confirms its efficacy. This new approach in elastography has the potential to significantly enhance patient care by advancing the accuracy and reliability of tissue elasticity assessments.

Multiphase flow and non-Newtonian fluid - Modelling and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MECHANISTIC MODEL FOR ICE DEPOSITION IN FREEZE DRYER CONDENSERS USING COMPUTATIONAL FLUID DYNAMICS

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ABSTRACT

This work presents a novel model for the deposition of ice in the condenser of a freeze dryer based on a computational fluid dynamics. The efficiency of the condenser has a significant impact on the efficiency of the overall process and the product quality. Therefore, a comprehensive understanding of ice deposition is essential for freeze-drying processes. The proposed condensation model integrates fundamental heat and mass transfer principles with the specific interactions that occur at the solid-vapour interface during ice deposition and further integrates these with transport phenomena in the condenser, including fluid flow, heat and vapour transport, which influence ice deposition kinetics. This is necessary because the pressure in the drying chamber can increase under various conditions, e.g. if the flow in the connecting duct is choked, if there is too much inert gas in the system or if the water vapour in the condenser is not sufficiently removed.

The vendor code Ansys Fluent with custom user-defined functions (UDF) were used to simulate the ice deposition, which was modelled as a volumetric sink of mass, momentum and energy. The ice deposition process is modelled as the one-way diffusion of water vapour. The numerical model was validated by an experimental comparison, which showed a high degree of agreement between the model predictions and the experimental data. The proposed model allows a comprehensive investigation of all potential causes and their mutual effects, making it a valuable tool for understanding and controlling the pressure dynamics in the system.

Using the validated model, a parametric study was performed by varying the temperature of the condenser walls, the mass flow rate of the sublimate and the mass fraction of the inert gas in the system. This study showed that energy consumption can be reduced in certain cases by selecting the optimum condenser wall temperature, as increasing the pressure in the condenser only slightly increases the pressure in the drying chamber.

The developed mechanistic model thus provides a deeper insight into the kinetics of ice deposition during freeze drying and enables process engineers to improve the design and operating parameters of the condenser to increase performance and product quality.

Nanomechanics and nanoscale thermal transport for new materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INVESTIGATION OF RESIDUAL STRESS MECHANISMS ON IRON SUBSTRATES DURING THE FORMATION OF DLC FILMS BY MOLECULAR DYNAMICS STUDY

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ABSTRACT

Due to their characteristics of low friction, high hardness, and wear resistance, diamond-like carbon (DLC) films are some of the hardest thin films expected to be applied to the mechanical sliding parts of automobiles. However, the poor adhesion of DLC films to substrates has caused delamination problems, particularly when used in high dynamic friction environments, and this limits the scope of their application. One of the main causes of delamination is high compressive residual stress, which originates from the deposition process. This cause-effect relationship is critical in understanding the practical application of DLC films. However, direct experimental observation of the generation of residual stress is difficult, as the phenomenon occurs at an atomic scale. In addition, the amorphous structure of DLC films precludes stress measurements by X-ray diffraction. To predict the local stress state of a film, a numerical simulation must be conducted. Accordingly, in this study, the residual stresses and structural changes of carbon bonds on iron substrates during the formation of DLC films were investigated through molecular dynamic simulations. Specifically, we conducted a detailed investigation of the manner in which carbon atoms form carbon bonds such as sp2 and sp3 on Fe-BCC substrates during the film formation process and how they contribute to the development of compressive residual stresses. Simulations showed that iron atoms ejected from the substrate penetrated the film and transformed the sp2 bonds into sp3 bonds in amorphous carbon, resulting in increased residual stress. The effects of the substrate material on the DLC-film bond structure and residual stresses are also thoroughly discussed through comparisons with previous studies.

MINIMAL SURFACES: WHAT ARE THEY GOOD FOR?

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ABSTRACT

“Economics, we all recite, deals with allocation of limited resources towards satisfaction of unlimited wants” [1]. But does that mean a good deal for you is a good deal for me? Minimal surfaces, so-called because of their local area minimization, are used as models in liquid crystals, foams, and block copolymers. Are they also energy minimizers? I will give examples of their use in these systems and raise the question, “are these really the best or are they just the best we can think of?”

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Advanced numerical techniques for fluid flow in porous media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICS-INFORMED NEURAL NETWORK VS FINITE ELEMENT METHOD FOR MODELING COUPLED WATER AND SOLUTE FLOW IN UNSATURATED SOILS

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ABSTRACT

Precise simulation of water and solute movement in unsaturated porous media is crucial in a variety of applications, including precision irrigation, and environmental conservation. The coupled model of water and solute flow involves integrating the Richards equation with the equilibrium advection-dispersion equation. The high nonlinearity of the Richards equation limits the availability of analytical solutions for the coupled system, especially with complex geometries and boundary conditions. Consequently, various numerical and data-driven approaches have been proposed (e.g., Haruzi and Moreno, 2023). In this study, we present physics-informed neural network (PINNs) solvers for the coupled system and provide a comparative analysis with the widely adopted finite element approach (FEM). The inputs for the PINNs solver consist of time and space coordinates, while the output provides the solution for the coupled system, encompassing water content and solute concentrations. To train PINNs solvers, random points are generated to calculate various loss functions, including the residual loss connected to the partial differential equations (PDEs), as well as initial and boundary losses. Two approaches are employed to satisfy the initial conditions: a soft approach, where the initial loss is integrated into the objective function for minimization, and a hard approach, where the output of the solver is transformed to fulfill both the initial conditions and the PDEs. Additionally, a comparison is made between a standard PINNs solver with a fixed activation function and an adaptive-based PINNs solver.

Numerical tests, encompassing both 1D and 2D scenarios, were conducted to assess the performance of the PINNs solver and its variants in comparison with the FEM. The PINNs solver exhibits a substantial increase in training time as the spatial dimension expands, in contrast to the FEM, which delivers results within minutes. Notably, the PINNs solver with adaptive activation and the hard implementation of initial condition constraints proves to be the most efficient in terms of accuracy. Conversely, the PINNs solver without adaptive activation requires more iterations to achieve comparable results. Soft implementation of initial conditions, in general, struggles to predict the initial condition near boundaries where Neumann conditions are applied. This underscores the need for further research to enhance the efficiency of PINNs solvers, enabling them to match the efficacy of standard numerical methods.

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Multi-scale, multi-rate damage and fracture: Models, experiments, and simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FAILURE ANALYSIS OF COMPOSITE LAMINATE BOLTED JOINTS: COMPARISON OF EXPERIMENTAL TEST RESULTS AND NUMERICAL ANALYSIS

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ABSTRACT

Recent developments in progressive failure simulation methods, based on increased computing capacities, provide the framework within which substantiation through numerical analysis, supported by experiments, can be envisaged. Nowadays, progressive damage models for the prediction of failure and failure modes are used [1, 2] and 3D finite element simulations are performed to describe and quantify composite material damage and to decrease the number of experiments required in the building block approach.

Here, a 3D multi-scale progressive failure approach developed at ONERA [3] has been implemented in the commercial calculation code Abaqus/Explicit, with an explicit solver. Explicit dynamics offers advantages over implicit modelling in solving large nonlinear problems. Different sources of non-linearities are considered by the OPFM model at the scale of the UD ply: (i) non-linear elasticity in the fibre direction, (ii) non-linear viscoelasticity of the matrix, (iii) matrix damage based on continuous damage mechanics and (iv) description of the sudden failure of the fibres with a softening law in the fibre direction regularised by a delay effect and delamination is described with cohesive zone elements. The model has been evaluated on different configurations provided by Airbus in order to predict accurately the final failure of composite structures subjected to in-plane or triaxial loading. First, some basic failure modes have been investigated on different configurations such as plain specimens and open-hole specimens in tension and compression on a CFRP thermoset UD Tape 194 gsm under prepeg format to evaluate the model. Then, damage and failures modes have been predicted on different composite laminate bolted joints in tension and compression. The simulation results will be compared with a large database coming from experiments provided by Airbus.

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PROBABILISTIC ENTROPY AND DISTANCE IN HOMOGENIZATION OF RANDOM MULTI-COMPONENT COMPOSITES

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ABSTRACT

The main issue is to use the apparatus of probabilistic entropy, and also probabilistic distance to perform uncertainty quantification related to effective characteristics of random composites built up with a few constituents. It is well known that uncertainty quantification is usually delivered in the literature using a few basic probabilistic characteristics like expectations, variances, and so on, so that a single function such as a probabilistic entropy may be an attractive alternative. Shannon entropy has been selected for this purpose, which is directly based on the given probability density function and which can be determined using a classical Monte-Carlo simulation scheme. Random composites under consideration have a perfect spatial distribution of the constituents, show some statistical scattering of the elastic characteristics, and also may exhibit some probabilistic interface defects in between the matrix and its reinforcements. Calculation of the effective composite characteristics is carried out with the effective modules method implemented in some Finite Element Method program, whose extension towards stochastic analysis is programmed using simulation, perturbation, and semi-analytical approaches. Additionally, probabilistic distance is analyzed in-between original material characteristics of such composite constituents and their effective parameters and this is completed using a relative entropy approach; the Bhattacharyya distance is selected for this purpose. Probabilistic distance enables us to determine the closest and the most distant material characteristics' probability distribution for the given component of the effective tensor. Therefore, it may serve as an alternative to traditional sensitivity analysis, not only for the homogenization procedure but as a general tool in stochastic computational mechanics.

Advanced computational mechanics based on data-driven techniques for structure, structural dynamics and aeroelasticity
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GNN-BASED REPRESENTATION FOR DESIGN OF THREE-DIMENSIONAL ROTOR BLADE STRUCTURES

Byeongju Kang[*1], Seongwoo Cheon[1], Haeseong Cho[1], Youngjung Kee[2] and Taeseong Kim[3]*

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ABSTRACT

Recently, there is active research on rotor blades in various fields such as advanced air mobility(AAM), wind turbine, military rotorcraft and more. In the structural design process of these rotor blades, dynamic characteristics analysis for the blades are necessary. This analysis process requires the cross-sectional stiffness of the blade, and the result of the analysis is utilized for assessing the structural integrity of the blade[1,2]. However, in the design process, recursive analyses are necessary whenever there is a change in the cross-sectional design. Therefore, the use of deep learning technique can be effective in reducing computational costs. Consequently, we are in the process of designing a prediction model that predicts the dynamic characteristics of the blade, and currently, we have developed two types of prediction models that predict the cross-sectional stiffness via structural properties of the blade cross-sections. The first prediction model, using multi-layers perceptron(MLP), has developed to investigate the feasibility of using deep-learning technique for predicting the cross-sectional stiffness of the blade. The input variables for the prediction model consider the position and thickness of the cross-sectional members, and the output variables are the cross-sectional stiffness terms. As an example problem for the training and verification of the prediction model, the r/R=0.3 cross-sectional geometry of IEA 15MW reference wind turbine blade[3] is used. The second model is developed to extend the predictive range along the spanwise direction of the blade in the MLP-based prediction model. Therefore, to additionally consider the cross-sections at r/R=0.1 and 0.5 in the example of the MLP-based model, graph neural network(GNN) is utilized. To evaluate the prediction results of the models, the coefficient of determination(R^2) is used. As the results of the MLP-based prediction model, the R^2 values for all stiffness terms are above 0.95. Also, the R^2 values of GNN-based prediction model are above 0.99 for all stiffness terms. As the future research, the development of blade dynamic characteristics prediction model via cross-sectional structural properties will be conducted.

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Architected materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CONTROLLING POISSON'S RATIO AND THERMAL EXPANSION IN A ROTATING RECTANGLE STRUCTURE COMBINED WITH BI-MATERIAL STRIPS

Duhwan Kang[*1], Jeong Min Hur[1] and Do-Nyun Kim[1]*

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ABSTRACT

Mechanical metamaterials have garnered significant attention due to their extraordinary properties surpassing natural limits, including negative Poisson's ratio (NPR) and negative coefficient of thermal expansion (NTE). Metamaterials with NPR contract laterally under axial compression, while those with NTE shrink when heated. Their unique properties make them promising for various applications including shape-morphing [1, 2].

Recently, various multifunctional metamaterials with both tunable Poisson's ratio (PR) and coefficient of thermal expansion (CTE) have emerged, rather than single-functional ones, to handle the complex thermo-mechanical loads. A common approach to achieving both properties involves combining auxetic structures with bi-material lattices. For instance, connecting a re-entrant structure auxetic to a bi-material triangle has shown tunable NPR and NTE [3]. However, prior works faced limitations in fully independent control of PR and CTE from negative to positive values, as the physical mechanisms for tuning PR and CTE are highly interrelated. The advent of solution to solve this problem will expand the potential uses in a wide range of applications and introduce novel functionalities.

This work introduces a novel meta-structure with independently tunable PR and CTE across a spectrum from negative to positive, demonstrating its controllability numerically and experimentally. Specifically, a rotating rectangle unit combined with alternating bilayer beams enables fully independent control of PR and CTE. Strategy for isotropic and anisotropic thermal expansion is also explored. Furthermore, we propose a novel application concept, the meta-surface, which offers diverse shape-morphing behaviors by exploiting the multi-functionality of the metamaterials when exposed to thermo-mechanical loads. Our advancements in the field of metamaterials may offer a robust foundation for applications capable of handling both mechanical and thermal loads, including shape morphing, stress mitigation, and smart actuation.

Acknowledgement
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Advances in numerical methods for solution of PDEs
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SUBSURFACE IMAGING OF STRUCTURES BY AN ELECTRICAL IMPEDANCE TOMOGRAPHY METHOD

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ABSTRACT

This study presents an electrical impedance tomography (EIT) method for subsurface imaging of structures in two dimensions. The proposed EIT method seeks to reconstruct the electrical conductivity profile of structures using measured electric potential differences at the boundary. The EIT method is based on a partial-differential-equation (PDE)-constrained optimization approach, which takes a complete electrode model (CEM) comprising the Laplace equation and boundary conditions for the electric potential difference as constraints. The finite element method was used to calculate the electric potential difference described by the CEM, and the accuracy of the forward solutions was validated by comparing them with ANSYS solutions. The inverse EIT problem seeks the optimal solution of the domain's electrical conductivity profile to minimize a Lagrangian functional consisting of a least-squares objective functional and a regularization term. By enforcing the stationarity of the Lagrangian, Karush-Kuhn-Tucker conditions comprising the state, adjoint, and control problems are derived. The three problems are iteratively solved in the reduced space of the control variable, the electrical conductivity, to image the structure. Numerical results show that electrical conductivity profiles, whether homogeneous or layered, could be effectively reconstructed using measured electric potential differences at the boundary. The relative error of the measured and calculated electric potential differences after the inversion was less than 1%, demonstrating the successful inversion of the measured data using the proposed EIT method.

Lattice Boltzmann modelling and study of complex flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LATTICE BOLTZMANN SIMULATION OF REACTIVE TRANSPORT IN COMPLEX FRACTURES

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ABSTRACT

Fractures play an important role in providing preferred flow pathways in low-permeability formations. They can improve gas production for shale reservoirs but can also increase the risks for leaking of carbon dioxide from geological storage sites. In addition, recent studies have shown that continuously created fractures are required to generate new mineral surfaces for sustainable carbon mineralization or subsurface clean hydrogen generation.

The fluid-mineral reactions, including dissolution or precipitation, can cause the alteration of fracture wall. Particularly, mineral dissolution (precipitation) can increase (decrease) the aperture size and hence the fracture permeability. While there have been a lot of two-dimensional studies on mineral dissolution in porous or fractured media considering resultant pore-structure, high-resolution pore-scale modeling study of reactive transport in three-dimensional fractures with evolving fracture geometry is scarce. Consequently, the complex coupled processes including fluid flow, solute transport, dissolution, precipitation, and evolution of pore structure are not well understood.

We are developing a high-performance computer code for simulating coupled fluid flow, solute transport, and chemical reaction in a single lattice Boltzmann method (LBM) framework. This allows for more accurate treatment of the coupled processes and improved computational efficiency. First we use LANL-developed open-source python library, Pysimfrac1, to create realistic fracture realizations of varying properties (e.g., fracture aperture and roughness). Then we perform a series of simulations of dissolution of the fracture wall by a reactant introduced at the entrance. We cover a wide range of Pe and Da numbers by varying flow rate and dissolution rate constant. Our preliminary results have shown that dissolution patterns highly depend on the combination of Pe and Da numbers. The results have also shown that roughness causes more surface area but lower velocity leading to the non-linear relation between roughness and effective reaction rate. We are carrying out more quantitative analysis of the effect of fracture characteristics on the effective dissolution rate and will present the results at the conference.

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Inverse and optimization problems for advanced materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SHAPE IDENTIFICATION OF SCATTERERS USING PERIDYNAMICS AND B-SPLINE PARAMETERIZATION

Sehyeon Kang[1], Hyun-Seok Kim[2] and Seonho Cho[1]*

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ABSTRACT

In this paper, we proposed a new shape identification method without a priori information about the scatterer. Shape identification, an inverse problem finding the configuration of scatterers by minimizing the discrepancy between real wave data with scatterers and estimated wave data, is investigated employing peridynamic theory and gradient-based optimization in plane elastic medium. To quantitatively measure the discrepancy, an error functional is defined as the L2 norm error obtained at several sensors located around the scatterers. The particle-based and non-local characteristics of the peridynamic theory enable the direct modeling of interface between scatterers and the medium, avoiding remeshing difficulties when employing conventional domain-based methods [1]. The boundary of scatterers is parameterized using a zero level of B-spline surfaces and determined by bond parameters in peridynamics material. The B-spline surface based parametrization enabled the precise boundary expression of the scatterers and topological changes during the identification process. Control points of the B-spline surfaces on the fixed grid are set as design variables. The design sensitivity of the error functional is efficiently obtained through an adjoint variable method, requiring only the solution of one additional adjoint equation to obtain the sensitivity [2]. The peridynamic adjoint sensitivity involving history-dependent variables in transient peridynamics is accurately obtained by using an identical path in both adjoint and response analyses. A gradient-based optimization scheme with an efficient adjoint variable method is utilized to determine the boundary of scatterers that minimize the error functional of discrepancy. Numerical examples of various geometry are presented to verify the accuracy and efficiency of the proposed method. The accuracy and efficiency of the proposed method could be further enhanced by implementing a multi-optimization scheme by increasing frequency inputs. This method can be extensively used in various fields (e.g. medical imaging, geometrical exploration, non-destructive testing) for accurate shape identification.

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Recent advances in partitioning method and interface mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ITERATIVE SOLUTION ALGORITHM FOR HIGHLY HETEROGENEOUS STRUCTURE BASED ON THE DISPLACEMENT-ONLY PARTITIONED FORMULATION

Seung-Hoon Kang[*1], SangJoon Shin[1], Kwang-Chun Park[2] and José A. González[3]*

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ABSTRACT

For the last few decades, a host of partitioning methods has been proposed for a parallel iterative solution algorithm. However, application of those for a heterogeneous system is still cumbersome, sometimes falling into a non-convergence. This paper suggests an alternative iterative algorithm based on the displacement-only partitioning (DP) formulation [1] for a highly heterogeneous material component. DP formulation handles the partitioned displacement as a fundamental variable, but does not include the interfacial variables, e.g., Lagrange multiplier. In addition to an implementation simplicity, such solution variable will maintain superiority in convergence and accuracy for the heterogeneity. The quasi-static structural analysis procedure based on the DP iterative algorithm will be demonstrated along with application of the various preconditioners, including the coarse space construction. Additionally, comparison against the traditional saddle-point and allied methods will be shown.

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Finite element techniques for wave simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ENHANCING LOW-ORDER DISCONTINUOUS GALERKIN METHODS WITH NEURAL ORDINARY DIFFERENTIAL EQUATIONS

Shinhoo Kang[*1] and Emil Constantinescu*[1]

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ABSTRACT

The growing computing power over the years has enabled simulations to become more complex and accurate.
However, high-fidelity simulations, while immensely valuable for scientific discovery and problem solving, come with significant computational demands. As a result, it is common to run a low-fidelity model with a subgrid-scale model to reduce the computational cost, but selecting the appropriate subgrid-scale models and tuning them are challenging. We have developed a novel continuous-in-time hybrid method that reduces the errors introduced by classical low-order discontinuous Galerkin (DG) discretizations. Our approach learns the missing scales of the low-order DG solver at a continuous level and hence improves the accuracy of the low-order DG approximations as well as accelerates the filtered high-order DG simulations. We demonstrate the performance of our approach through Taylor–Green vortex examples at different Reynolds numbers and times, which cover laminar, transitional, and turbulent regimes. The proposed method not only reconstructs the subgrid-scale from the low-order (1st-order) approximation but also speeds up the filtered high-order DG (6th-order) simulation by two orders of magnitude.

Computational methods in environmental fluid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE MODELING FRAMEWORK USING ELEMENT-BASED GALERKIN METHODS FOR SIMULATION OF THE MOIST ATMOSPHERE

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ABSTRACT

Atmospheric flows involve a broad spectrum of spatial and temporal scales and their multiscale interactions, encompassing large-scale convective processes and small-scale moist processes. Therefore, one of the main challenges for simu- lating atmospheric flows is to resolve the processes across various scales, ranging from global circulation to precipitation microphysics. The multiscale modeling framework (MMF) [1, 2] uses local fine grids to explicitly resolve phenomena at distinct scales using different grid resolutions within a global circulation model (GCM).

This talk adapts the MMF approach to model moist atmospheric limited- area (mesoscale) simulations. The MMF resolves the large-scale convection us- ing a coarse grid while simultaneously resolving local features through numerous fine local grids, and seamlessly coupling them. Both large- and small-scale processes are modeled using element-based Galerkin methods [3] with high-order basis functions. Coupling of the two models are achieved in either a column- based or block-based manner. Consequently, the atmospheric flow model is informed by the local microphysics. The proposed method is tested in 2D and 3D limited-area weather problems involving storm clouds, i.e., squall line and supercell simulations.

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Computational methods in environmental fluid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN IMPLICIT DISCONTINUOUS GALERKIN METHOD FOR TWO-DIMENSIONAL SHALLOW WATER EQUATIONS

Younghun Kang[1], Mark Loveland[2], Corey Trahan[2] and Clint Dawson[1]*

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ABSTRACT

Two-dimensional shallow water (2D SW) equations are widely applied for various physical phenomena such as global tides and storm surges. Numerical models have been developed using various discretization schemes. This work focuses on the 2D SW Adaptive Hydraulics (2D SW AdH) model, which is developed by U.S. Army Corps of Engineers ([1]). The 2D SW AdH model is an unstructured, implicit, Petrov-Galerkin finite element method model. As the name implies, the AdH model is capable of adaptivity in both space and time, and the performance of AdH has been demonstrated with various test cases (see [1]). In this work, we develop an implicit discontinuous Galerkin method for 2D SWE (2D SW AdH-DG) within the 2D SW AdH framework. In the 2D SW AdH-DG model, 2D SW equations are spatially discretized using local discontinuous Galerkin method and Local Lax-Friedrichs flux is utilized for numerical flux. The 2D SW equations are temporally discretized using finite difference method, which is between first- and second- order scheme based on user-defined parameter. The model is verified with fully wet domains and the results are compared with 2D SW AdH model.

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Topology optimization for additively manufactured metamaterials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A METHOD OF SUCCESSIVE ITERATION OF ANALYSIS AND DESIGN FOR LARGE-SCALE DYNAMIC TOPOLOGY OPTIMIZATION

Zhan Kang[*1], Yixiao Zhu[1] and Xiaopeng Zhang[1]*

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ABSTRACT

Large-scale dynamic topology optimization of structures and metamaterials considering natural frequencies, transient responses or wave propagation properties is a challenging task due to the high computational cost required by the iterative computation of the dynamic performances and their sensitivities. This presentation introduces recent developments of a new framework based on successive iteration of analysis and design (SIAD) for finding high-quality solutions at affordable computational costs. In the original SIAD method for natural frequency-related topology optimization problems, the eigenvalue solution routine is integrated into the optimization iterations to achieves sequential approximations of the eigenpairs along with the structural design evolution, thus avoiding the time-consuming eigenpair analysis in each optimization iteration. A multi-step relay approach has been developed to further enhance the computational efficiency, in which the optimization process starts from a relatively coarse finite element discretization, and then gradually refined meshes are used to improve the design resolution. For a given level of mesh resolution, by sequentially solving the optimization problem and projecting intermediate designs and the corresponding approximate eigenmodes from a coarser mesh onto finer meshes, the proposed multi-step relay method can further reduce the computational cost and yield high-resolution solutions in the final design. This method can be used to solve natural frequency maximization topology optimization problems with millions of degrees of freedom on a desktop workstation, and is much more efficient than the conventional double-loop method. The SIAD method has also been combined with a quasi-static response-enhanced mode displacement method and thus extended to topology optimization of transient responses, in which the approximate eigenmodes and quasi-static responses are used as the model reduction basis for each intermediate design. Numerical examples show that the method significantly improves the efficiency of dynamic topology optimization.

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Modeling and simulation of coupled processes in geological media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HYBRID ISOGEOMETRIC - FINITE ELEMENT MODELLING OF COUPLED THERMO-HYDRO-MECHANICAL DEFORMATION OF FRACTURED MEDIA IN THREE DIMENSIONS

Ellya Kanimova[*1], Adriana Paluszny[1], Marco Paluszny[2] and Robert Zimmerman[1]*

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ABSTRACT

Monolithically coupled partial differential equations for thermo-poro-elastic deformation of fractured rocks are solved using the finite element method. The rock matrix is assumed to be linear elastic and isotropic, Darcy fluid flow is assumed in the matrix, and laminar fluid flow is assumed in the fractures. The volume is discretised by tetrahedral and hexahedral meshes, using quadratic or mixed Taylor-Hood elements for improved stability. Fractures nucleate in response to the local accumulation of damage. Fractures are sub-dimensional features represented by NURBS surfaces to capture the geometry; on these, a hybrid sub-dimensional isogeometric solution is embedded and coupled with a volumetric finite element solution. These solutions locally interpolate the fields, yielding a dual representation on the fracture surface and leading to smoother approximation of stress intensity factors around the fracture tips. Growth angles are computed using the Richard method based on the stress intensity factors, resulting in crack propagation vectors that modify the discrete geometry of the resulting non-planar fractures. After each growth event the geometry and discretisation are regenerated and optimised to the new geometry. Examples of coupled deformation and crack growth are shown in the context of fracturing under coupled thermo-poro-elastic processes. Resulting fracture patterns are compared against experimental and field observations.

Emerging frontiers and methods in digital manufacturing: Modeling, simulation, and beyond
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DIGITAL TWIN INFERENCE FROM MULTI-PHYSICAL SIMULATION DATA OF ADDITIVE MANUFACTURING PROCESSES: PROOF OF CONCEPT STUDY

Maximilian Kannapinn[*1], Felix Rutsch[1] and Oliver Weeger[1]*

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ABSTRACT

A digital twin is a virtual representation that accurately replicates its physical counterpart, fostering bi-directional real-time data exchange throughout the entire process lifecycle. This study explores the integration of digital twins into additive manufacturing processes, particularly focusing on lattice structures. In additive manufacturing, digital twins help to control the process better and progressively react to unplanned processing results. Employing faster-than-real-time and highly accurate surrogate models enables the prediction of altered structural properties, facilitating on-the-fly re-optimizing the ongoing manufacturing process to still achieve desired structural outcomes. Consequently, this approach contributes significantly to realizing the first-time-right paradigm in additive manufacturing.

The foundation of successful digital twin derivation lies in the physics-based modeling of the additive manufacturing process. Predicting final structural properties necessitates mapping input parameters to potentially non-linear material properties [2]. However, a challenge arises from the need to provide faster-than-real-time replications of these mappings through simulations, particularly as the complexity and computational cost of multi-physical simulation models increase. This study addresses the aforementioned challenge by presenting an efficient training methodology for digital twins, utilizing only minimal training datasets extracted from multi-physical simulation models. An efficient design of experiments aids in selecting representative training data, ensuring minimal test error on the twin when applied to pertinent test data. The proposed solution includes a comprehensive software suite that automates simulation model management, training data selection, reduced-order model derivation, and integration of digital-twin-based control techniques into a unified framework. The versatility of this framework, specifically designed for seamless integration with various simulation models, was initially exemplified through its application in autonomous thermal food processing [1]. Remarkable efficiency gains are achieved. Computational efficiency is demonstrated by characteristic solution times of one-tenth of a second, imposing negligible processing costs on a single-core processor. The framework showcases practical viability by predicting field data with 4649 spatial points and one hour of real-time processing outputs within less than 0.5 s.

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Microstructures of chemically complex materials and their impacts on material properties from multiscale simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THEORETICAL INVESTIGATION FOR THE HYDROGEN EVOLUTION REACTION ENHANCEMENT OF THE TWO-DIMENSIONAL MOS2 VIA LITHIUM INTERCALATION

Jui-Cheng Kao[12], Yu-Chieh Lo[1] and Chun-Wei Pao[2]*

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ABSTRACT

Hydrogen (H2) is considered a potential energy carrier for the next generation due to its high energy density, high combustion efficiency with zero emission, and nontoxicity. Among the various explored catalysts, two-dimensional (2D) transition metal dichalcogenides (TMD) have emerged as the state-of-the-art candidates for electrocatalytic H2 production beyond the traditional noble metal catalyst (Pt, Pd) owing to their intriguing electronic properties, large surface area, and relatively low fabrication cost. However, the insufficient utilization of active sites (edge), low electrical conductivity, and poor durability limit their intrinsic activity and the developed potential. To overcome the aforementioned issues, introducing atomic-scaled intercalation in the layered 2D materials is a powerful strategy. In this study, we introduce lithium (Li) as intercalant to promote the hydrogen evolution reaction (HER) activity and the structural stability for both the 2H- and 1T-MoS2 materials, which are revealed by the density functional theory (DFT) calculations. Our calculation results show that Li intercalation will enhance adsorption strength of H* on 2H-MoS2 basal plane, and the optimal adsorption site of H* will be changed by the position of intercalant. The computed Gibbs free energy of the HER (ΔGH*) indicates drastic enhancement of the HER reaction activity at the basal planes by Li intercalation. As for 1T-MoS2, the HER performance at the basal plane will also be promoted under the certain intercalant concentration. Such an activity enhancement can be attributed by the charge transfer between the host material and intercalant, and subsequently the rearrangement of electron density distribution for the surface atoms. Moreover, the intercalation energy demonstrates the structural stability of both the 2H- and 1T-MoS2 are improved after Li intercalation, especially for 1T phase. Even for the maximum intercalant concentration (LiMo2S4), it still yields the negative value of intercalation energy (-0.702 eV and -1.714 eV for 2H- and 1T-phase, respectively), implying that intercalated MoS2 are thermodynamically stable. In summary, both the HER activity at the basal plane and structural stability of layered MoS2 materials can be substantially promoted via Li intercalation. Hence, we demonstrate that intercalation is the effective methodology to enhance the HER performance on the basal plane of 2D material as the alternative way to the defect engineering.

Enabling technologies for digital twins: Model reduction and scientific machine learning
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CONCEPTUAL DESIGN FOR PREDICTIVE DIGITAL TWINS: CONCEPTS, TOOLS, AND TECHNIQUES TO ENSURE FITNESS FOR PURPOSE

Michael Kapteyn[1] and Karen Willcox*[1]

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ABSTRACT

Advancements in computational technologies, including reduced-order modeling (ROM), uncertainty quantification (UQ), and scientific machine learning (SciML), offer significant potential for improving the accuracy, efficiency, and robustness of digital twins. However, adopting a systems engineering perspective reveals that the design of a digital twin is a multi-objective optimization problem, with inherent tradeoffs across multiple axes such as investment in technology development, computational costs, implementation complexity, accuracy, reliability, and robustness [1]. Thus, the challenge lies in making data, modeling, and algorithmic choices that align with the application area, decision-support context, and computational constraints, so as to ensure that the resulting digital twin is “fit-for-purpose” [2].

In this presentation I will discuss the above challenges, highlighting the understudied conceptual design phase in digital twin development and drawing parallels to the multidisciplinary engineering design optimization of physical systems. I will then present ongoing work to address these challenges by developing conceptual design tools for digital twins. First, I will build upon the mathematical abstraction for digital twins established in prior work [3] to develop a definition language for digital twin architectures. I will then discuss tools and techniques for assessing the performance characteristics of different digital twin architectures. The goal of this work is to empower digital twin designers to navigate and explore tradespaces over various architectural decisions, develop a fit-for-purpose digital twin architecture, and derive requirements for the various models and algorithms that comprise the digital twin. Such requirements can then drive the research, development, and adoption of computational technologies such as ROM, UQ, and SciML. I will illustrate these concepts and developments in the context of ongoing work within the Willcox Research Group, showcasing digital twin applications ranging from cancer patients to space satellites.

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Modeling and inverse design of architected materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MECHANICS OF 3D INTERTWINED LATTICES

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ABSTRACT

Architected truss lattice materials have recently enjoyed popularity due to advances in 3d-printing, and they are being increasingly used in several applications. In particular, intertwined lattices have emerged as a new family of architected materials, which replace conventional struts with intertwined or woven strands. By extending principles of weaving, typically found in two-dimensional fabrics, to bulk three-dimensional architectures, these materials promise interesting properties.

First, we an efficient an efficient numerical framework for computing the effective mechanical response of periodic intertwined materials, relying on a nonlinear beam formulation, and a conforming frictional beam-to-beam contact algorithm, embedded into a computational homogenization framework. Next we discuss how we can explore the design space of such materials, specifically the generation of the topology and geometry of intertwined unit cells, by casting it into an optimization problem. We quantify the effect of unit cell topology on the effective mechanical response of an inertwined unit cell, and present additional applications where we design architectures with properties such as tunable elasticity and high energy absorption. Lastly, we cover the experimental calibration and validation of the model, with experiments on 3d-printed intertwined materials.

PSE (Problem Solving Environment)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RELATIONSHIP BETWEEN PERFECTIONISM TENDENCY AND SPORTS INJURIES

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ABSTRACT

Most of the world's top athletes have a “perfectionist mindset," which suggests a relationship with poor health and maladjustment. Additionally, as Japan's Internet usage rate (SNS usage rate) continues to increase, opportunities to compare oneself with others in SNS activities will increase significantly. Therefore, it is suggested that in the future in Japan, the number of young people with “perfectionist thoughts" will increase, as well as the number of athletes with perfectionist thoughts. Furthermore, “sports injuries" are one of the events that can disrupt an athlete's competitive life, and even these “sports injuries" can be seen to be associated with poor health and maladjustment. However, there is currently very little research linking “perfectionist tendencies" and “sports injuries." A survey was conducted among athletes and former athletes affiliated with University A. There were three scales/questionnaires used: one was the four factors that emerged from a multifaceted view of "self-oriented perfectionism," which is one of the perfectionist ideologies, "setting high goals for oneself." The “new multidimensional self-oriented perfectionism scale (MPPS) " includes “desire for perfectionism ", “personal standard", “concern over mistakes ", and “doubting of actions ". The second is the “scale for Assessing in injured Athletes," which includes “development of self-understanding" and “expanding and deepening subjective considerations," which are two important factors for returning to competition. Finally, we used “sports-related questions" that asked participants about their competitive history, whether they had ever been injured, the details of their injuries, and the causes of their injuries. As a result, the “personal standard " included in the “new multidimensional self-oriented perfectionism scale " was found to be positively correlated with “development of self-understanding" and “expansion and deepening of the scope of consideration. In addition, in a question related to sports, it was suggested that one issue with club and sports activities in Japan is that injuries are increasing due to “over-practicing." In the future of athlete education in Japan, it will be necessary not only to focus on athletes' physical aspects and performance, but also to conduct psychological tests and understand their personality traits. As a future issue, what kind of research results can be obtained when there is a strong tendency for other perfectionism such as "other-oriented perfectionism" or "socially-oriented perfectionism"? Both findings suggest an increase in knowledge about how to avoid "over-training" and improve athletes' abilities.

Advances in computational biomechanics and mechanobiology
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A COMPUTATIONAL PRESTRESSING ALGORITHM FOR BIOLOGICAL TISSUES: APPLICATION TO THE AORTA AND CONSEQUENCES ON GROWTH AND REMODELING

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ABSTRACT

In computational biomechanics, accurately modeling biological tissues presents a unique challenge, particularly for patient-specific applications. Classical continuum mechanics and finite element methods usually rely on known stress-free reference configurations, a condition not met when modeling tissues reconstructed from in vivo medical images. The identification of the stress-free configuration is an inverse problem with high computational costs, especially when applying the constrained mixture theory, which considers varied material properties and homeostatic stretches in different tissue constituents [1]. Addressing this, we propose a novel prestressing methodology designed to approximate the in vivo residual stress field or identify its stress-free configuration.

Our approach, inspired by thermal contraction principles, innovatively updates the deformation gradient incrementally at each integration point, to minimize deviation of the loaded geometry from the actual in vivo geometry. Implemented in the commercial finite element solver Abaqus through the UMAT subroutine, our algorithm demonstrates rapid convergence in complex patient-specific geometries, including human ascending and abdominal aortas.

By successfully identifying the in vivo residual stress map as an initial condition, we explored arterial wall growth and remodeling under various mechanical stimuli. By maintaining the mechanobiological equilibrium in our finite element simulations [2], we measured changes in wall morphology and tissue composition in response to alterations in internal pressure and axial tension. Notably, our findings highlight the importance of incorporating residual stresses in simulations, as evidenced by comparing results obtained with and without prestressing.

This research advances computational biomechanics and paves the way for more precise patient-specific simulations, essential for understanding and predicting tissue behavior under both physiological and pathological conditions.

Keywords: Inverse finite element, Prestressing, Constrained mixture, growth & remodeling, Patient-specific modeling.

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Immersed-boundary variational methods: Theory, data structures, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMPLICIT GEOMETRIC REPRESENTATION FOR THE CONSTRUCTION OF OCTREE-MESHES FOR FINITE ELEMENT ANALYSIS

Samundra Karki[*1], Mehdi Shadkhah[1], Adarsh Krishnamurthy[1] and Baskar Ganapathysubramanian[1]*

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ABSTRACT

Recent advancements in 3D surface representation have witnessed a shift toward using neural implicit surfaces, which exploit the capabilities of neural networks or multi-layer perceptrons (MLPs) to represent complex geometry. Specifically, these implicit representations use the signed distance to query the occupancy information at a 3D location, departing from traditional ray tracing methods used in mesh-based geometry. MLP-based representations can capture geometry with arbitrary topology, provide multi-resolution control, and maintain an efficient memory footprint [1]. Despite the versatility of implicit representations, their application in computational analysis remains largely unexplored.

In this work, we explore using neural network architectures for constructing octree meshes for complex geometries. We explore different loss functions optimized for reconstructing the signed distance fields of complex geometries. The trained MLPs are integrated with an octree-based Finite Element Method (FEM) solver (Dendrite-kt), which can be directly used for fluid flow simulations over complex geometries [2]. We empirically show this methodology is faster than the conventional ray tracing algorithms used for octree construction, especially for geometries consisting of a large number of triangles. The streamlined structure of MLP architectures ensures that they can be efficiently embedded within a single CPU node, markedly enhancing the computational tractability and scalability of high-performance simulations. We have validated these methods to confirm that these MLP-driven models attain a level of precision analogous to that of established ray tracing techniques, thereby preserving the accuracy of previously validated simulation results.

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Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A GENERALIZED HOMOGENIZATION APPROACH TO DESCRIBE THE ORIENTATION DYNAMICS OF FIBER SUSPENSIONS

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ABSTRACT

Predicting the evolution of fiber orientation during mold filling of fiber suspensions is a computationally challenging task. To keep the computational effort reasonable, the averaging concept of fiber orientation tensors [1] is used in engineering practice. The fiber-induced anisotropic viscosity of the suspension leads to a so-called flow-fiber coupling, i.e. the fiber orientation influences the flow field and vice versa. In this context, the anisotropic viscosity of the fiber suspension must also be considered in the fiber orientation evolution equation beyond the standard kinematic terms in order to model the orientation dynamics comprehensively.

In this contribution, a generalized evolution equation for the fiber orientation tensor of arbitrary order is formulated that takes into account the microstructural anisotropy of the fiber suspension. This computationally efficient coarse-grained formulation is based both on the consideration of a single fiber at the microscale and on an upscaling of the respective local spin tensor. In this context, a previous work [2] is generalized and the corresponding methodology of using a linear homogenization approach is applied. The derived fiber-fiber interaction term is discussed as a micromechanical convergence criterion of the underlying integral operator. It is discussed how the special case of Jeffery's equation [3] follows from this general formulation. Beyond Jeffery's approach, the generalized evolution equation is specified for additional mean-field models. In this context, a novel equation is presented to describe the evolution of the fiber orientation tensor of arbitrary order depending on the spatial fiber distribution.

The prediction of fiber orientation in a shear flow is investigated with respect to different mean-field models. It is shown that the type of mean-field model, the fiber volume fraction, and the spatial fiber distribution significantly affect the orientation dynamics of the fiber suspension. The computational complexity of the considered mean-field models is discussed in terms of constraints on the choice of an efficient closure method and numerical integration on the unit sphere. It is found that there are significant differences between the considered models and that an encapsulated numerical integration leads to an unacceptably high computational cost.

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Data-driven methods for modeling complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CONSTRAINED OPTIMIZATION OF SENSING IN NUCLEAR REACTORS UNDER UNCERTAINTY

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ABSTRACT

The optimal placement of sensors with respect to restrictive spatial constraints is essential for the reconstruction of nuclear reactor flow fields and online calibration of nuclear digital twins. We develop a data-driven optimization technique for sensor placement, which aims to minimize reconstruction error of flow fields under sparse, noisy sensor measurements. The proposed greedy algorithm optimizes sensor locations over high-dimensional grids, adhering to spatial and dynamic constraints based on operating tolerances of sensors. We apply the algorithm to the Out-of-Pile Testing and Instrumentation Transient Water Irradiation System (OPTI-TWIST) prototype capsule, which is electrically heated to emulate the neutronics effect of the nuclear fuel. The resulting sensor-based temperature reconstruction within OPTI-TWIST demonstrates minimized error, provides probabilistic bounds for noise-induced uncertainty, and establishes a foundation for communication between the digital twin and the experimental facility.

Physics-based data-driven modeling and uncertainty quantification in computational materials science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NOVEL, CONSISTENCY-BASED METRIC FOR PROBABILISTIC REMAINING USEFUL LIFE MODEL SELECTION

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ABSTRACT

Physics-based, data-driven, and hybrid models are used for remaining useful life (RUL) prediction in various engineering applications. These models are usually calibrated/trained using data obtained from accelerated material failure tests. The calibrated/trained RUL model is, however, used to predict material performance under normal operating conditions. Normal operating conditions are significantly different than the accelerated test conditions, and material failure data under normal operating conditions is not available in many cases. To tackle the problem of choosing the best probabilistic RUL prediction model for such extrapolation situations, a model consistency-based metric is proposed in this research. The proposed metric evaluates the inconsistency in the probabilistic RUL prediction, where inconsistency is measured using the statistical distance between probability distributions of RUL over the probability distribution of normal operating conditions. A two-step approach for model selection is proposed. In the first step, model validation is performed using previously developed metrics and accelerated test data. In the second step, model consistency is evaluated for the normal operating conditions. The model with superior performance in both these steps is chosen to be the best RUL prediction model. The proposed methodology is demonstrated using five RUL models for polyethylene (PE) pipes. Bayesian inference is used to calibrate these models using accelerated test data. The proposed two-step model selection methodology is compared against traditional model selection methods (goodness of fit, model complexity and information theoretic metrics). The proposed methodology is applied to different normal operating conditions, and it is shown how different models could be more consistent in predicting PE pipe RUL under these circumstances. It is shown that the proposed additional consistency criterion is useful for selecting the best RUL prediction model in these, practically relevant, scenarios.

Performance-portable algorithms for unstructured mesh applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HPC CONSIDERATIONS FOR GLOBAL KM-SCALE EARTH SYSTEM MODELS

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ABSTRACT

Efforts are underway in the weather and climate modeling community towards substantial horizontal resolution refinement of global atmosphere GCMs to km-scale in order to explicitly resolve some of the small-scale convective cloud processes and provide more realistic local information on climate change and extreme weather events. At the same time, Exascale HPC systems have arrived and in most cases are powered by GPU accelerator technology that offers opportunities in practical simulation turn-around times balanced with efficiency in energy consumption. High-resolution model developments driven by the need for global storm-resolving simulations featured in projects such as DNA Climate, DYAMOND, SCREAM, nextGEMS, and EXCLAIM have motivated NVIDIA collaborations in GPU development of Exascale-ready AGCMs for next-generation Earth system models. This talk will describe the challenges and expectations for the directions of accelerator-based programing methods, GPU strong-scaling experiences with km-scale AGCMs, and large data handling for post-processing and visualization; and examine the requirements to develop Earth system digital twins from km-scale models as proposed in programs like the EU Destination Earth and NVIDIA Earth-2.

Data-driven modeling and design of materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN EXPLORATION OF STRUCTURE-PROPERTY LINKAGES AND INVERSE DESIGN OF MATERIALS

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ABSTRACT

Being able to design, e.g., the microstructure of a material to achieve a desired behavior is a key enabler for innovation. To achieve this goal, knowledge about the influence of the local material structure on the mechanical properties of the material, e.g. measured in terms of stiffness, strength or ductility, must be acquired. Ideally, experiments and simulation results are combined to build structure-property linkages. The key challenge is then to invert this knowledge to find a material structure for a desired set of material properties. This process is known as inverse design.

While surely inverse design is challenging, even the forward prediction of SP linkages using multiscale simulations of complex microstructures is still a demanding task. The difficulties lie in (i) describing the features of the local material structure, (ii) reconstructing plausible 3D statistically representative volume elements (SVEs), e. g., from 2D slices like microscopy images, (iii) modeling the complex and non-linear effective constitutive response and (iv) using it in an efficient multiscale scheme.

In this contribution, we present recently developed methods that aim at addressing these issues and it is shown how to integrate them in an efficient workflow. Descriptors are employed to characterize complex microstructures. Examples of such descriptors are volume fraction, generalized spatial n-point correlations or Gram matrices of pre-trained convolutional neural networks. Corresponding SVEs are generated using differentiable microstructure characterization and reconstruction (DMCR). An advantage of DMCR over similarly efficient reconstruction algorithms is that it allows to prescribe generic high-dimensional microstructure descriptors as long as they are differentiable. The reconstructed structures are then used for numerical simulation and effective properties are obtained from homogenization techniques. Together with the descriptors of the local material structure, SP linkages are set up.

As engineering data, including the SP linkages, are generally costly to generate, inverse design has to cope with scarce data. We therefore employ a Bayesian optimization approach and it is shown that significantly less data are needed in comparison to classical sampling procedures and alternative inverse design methods which is due to the iterative data augmentation. The approach is demonstrated for spinodoid metamaterials. In future work, the active learning augmentation loop could be applied to a broader range of materials.

New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN TOPOLOGY OPTIMIZATION FOR NON-RELAXED STRESS MINIMIZATION PROBLEMS

Misato Kato[1], Taisei Kii[1], Kentaro Yaji[1] and Kikuo Fujita[1]*

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ABSTRACT

In structural design, stress concentration is a crucial consideration due to its significant influence on the strength of the structure. Consequently, there are many studies related to topology optimization for the maximum stress minimization problem. However, the following issues remain with conventional topology optimization methods.
Firstly, gradient-based methods are commonly employed for topology optimization, but they require transforming the original problem into any differentiable pseudo-problem through relaxation techniques. These relaxation techniques include grayscale, approximation of maximum stress, and relaxed stress. Although these techniques are essential for the gradient-based methods to solve maximum stress minimization problems, these methods only solve a pseudo-problem.
The second difficulty is stress concentration caused by structured mesh. The structured mesh is generally used in topology optimization, but it creates staircase-like boundaries that will have stress concentrations. Generally, after optimizing with structured mesh, post-processing such as smoothing is applied to the optimized designs, and they are evaluated by stress analysis using body-fitted mesh. However, the maximum stress values can change significantly with slight structural modifications through these post-processing steps.
To overcome these issues, we propose a new approach to treat the non-relaxed maximum stress minimization problems and optimize them based on evaluation using body-fitted mesh. In this study, we focus on data-driven multifidelity topology design (MFTD) [1], which is a non-gradient topology optimization approach using a deep generative model. Its concept involves dividing the design problem into low-fidelity optimization and high-fidelity evaluation, iteratively updating solutions based on Evolutionary Algorithms (EAs). We generate multiple diverse and reasonable initial solutions through conventional gradient-based topology optimization using relaxation techniques as the low-fidelity optimization model. Their objective values are evaluated with the exact analysis model using body-fitted mesh as high-fidelity evaluation, and iteratively update the solutions by using a deep generative model as a crossover-like operation in EAs.
We apply the proposed approach to L-bracket and compliant mechanism design problems. We obtain initial solutions by solving the gradient-based topology optimization using the p-norm stress measure and solve the non-relaxed maximum stress minimization problems. The optimized designs obtained through data-driven MFTD are more rounded structures that alleviate stress concentration and completely dominate the initial solutions, demonstrating the effectiveness of our proposed approach.

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New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DENSITY-BASED TOPOLOGY OPTIMIZATION FOR ITR-FREE THERMAL CLOAK

Seitaro Kato[1], Kohei Takejima[1], Yugo Kondo[1] and Garuda Fujii[1]*

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ABSTRACT

Thermal cloak was proposed as an analogy to invisibility cloak in thermotics and it has been developed as a metadevice to make an obstacle thermally undetectable by controlling temperature distribution around the obstacle as if nothing is present. Thermal cloaks are usually composed of thermal metamaterials with artificial microstructures that provide the anisotropic/isotropic heat conduction required by transformation thermodynamics. Besides, a thermal cloak composed of naturally available isotropic materials has also been proposed such as bilayer cloaks. Topology optimization is promising numerical approach to optimize the distribution of isotropic materials around an obstacle for designing thermal cloaking structures. Topology optimization based on level set, density, and homogenization methods have been implemented, respectively, for the optimal design of thermal cloaks.

The above previous works attempted to compose thermal cloaks more than two materials with different thermal conductivity. It is well known that the effect of interfacial thermal resistance (ITR) between two different materials increases as the scale decreases and has a significant impact on device performance in nanoscale heat transfer. Similar problems have been reported for thermal cloaking, and it is necessary to construct a thermal cloak using only one material to prevent degradation of thermal cloaking performance due to ITR.

To overcome the problem on the ITR, ITR-free thermal cloak was proposed. Effective thermal conductivity in two-dimensions is adjusted by changing the height of the host material. The height distribution is set based on the bilayer scheme to achieve a two-dimensional thermal cloak.

In this work, we attempt to optimize the structural topology of ITR-free thermal cloak by a density-based topology optimization. Thermal cloaks are usually composed of more than two materials, but the presented ITR-free thermal cloak is composed of single material by changing the structural height of the host material. The local height of the host plate is optimized as continuous design variable, and hence, grayscales are interpreted as a structural height of host structure. Optimal configurations obtained exhibit good cloaking performance, and we investigate how the cloaking performance changes when the maximum height of the host material and volume constraint in the fixed design domain are changed.

Large-scale structural and fluidic topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LARGE-SCALE UNSTEADY FLOW TOPOLOGY OPTIMIZATION WITH HIERARCHICAL CARTESIAN MESH METHOD AND ITS PARALLEL PERFORMANCE EVALUATION

Ryohei Katsumata[*1], Koji Nishiguchi[1], Hiroya Hoshiba[1] and Junji Kato[1]*

[1]Nagoya University

ABSTRACT

In recent years, topology optimization methods have been applied not only to structural problems but also to fluid flow problems. Most of the previous studies assume steady flows or two-dimensional flows. In contrast, this study focuses on topology optimization for unsteady flows[1], which are more general from an engineering point of view. However, topology optimization for unsteady flows involves solving the governing and adjoint equations of a time-evolving system, which is computationally more expensive than for steady-state flows. Thus, a method suitable for large-scale computation, i.e., a numerical method with high parallel efficiency, is indispensable to perform topology optimization with a finer computational mesh. Therefore, we propose a large-scale unsteady flow topology optimization method based on the building-cube method (BCM)[2], which is one of the hierarchical Cartesian mesh methods. The BCM is suitable for massively parallel computing and has been confirmed to have excellent scalability[3]. The governing and adjoint equations are discretized by a cell-centered finite volume method based on the BCM. The sensitivity of the objective function is obtained by the continuous adjoint method. In the presentation, we discuss the applicability of the proposed method to large-scale computation through several examples of topology optimization and evaluation of computational efficiency by weak scaling.

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Microstructures of chemically complex materials and their impacts on material properties from multiscale simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTATIONAL MODELING OF NANOPARTICLE-COATED SURFACES FOR RENEWABLE ENERGY APPLICATIONS

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ABSTRACT

Using first-principles calculations based on density functional theory, we investigate the efficiencies of hydrogen evolution reaction (HER) and CO2 photoconversion on nanoparticle-coated surfaces. Effects of hydrogen spillover, nanoparticle-substrate interaction and material configuration are addressed. Particularly, our calculations show that the Pt/ZnO heterostructure has a good performance for the HER process [Int. J. Hydrogen Energy 47, 40768 (2022)], the adsorption energies of H and CO on TiO2 can be the electronic structure-based descriptors of Pt/TiO2 heterostructures for photocatalytic CO2 conversion to distinguish between H2 evolution and CH4 formation [Appl. Surf. Sci. 635, 157678 (2023)], and the synergistic effects of multiple-oxides/metal composition enhance the disassociation of H-OH and the evolution of H* to gaseous H2, thus achieving high activity of a composition design for noble metal free catalyst [ChemSusChem 16, e202300820 (2023)].

Minisymposium in honor of Prof. Yannis Kallinderis's 60th birthday: Progress of Unstructured grid based CFD, hybrid mesh generation and adaptation, and parallel supercomputing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A COMPACT SIXTH ORDER FINITE DIFFERENCE SCHEME FOR THE 3D POISSON EQUATION

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ABSTRACT

We present a sixth order finite difference scheme for Poisson's equation when discretized with the compact 27-point stencil based on Mehrstellen corrections of the forcing function term f. Our approach results in a sixth order accurate solution error as opposed to a fourth-order error imposed by the classical Mehrstellen correction for the 19-point and 27-point stencils. The present study is a continuation of former work of Spotz and Carey (1996) on compact finite difference schemes for Poisson's equation where sixth order convergence may be obtained under the assumption that the fourth order derivatives of f are determined analytically. Specifically, we show that sixth order convergence can still be attained when only values of f at grid points are available. The sixth order Mehrstellen scheme is further coupled with a Method of Local Corrections (MLC) 3D Poisson solver improving to sixth order accuracy the results reported in Kavouklis and Colella (2019). The MLC test case considered involves an adaptive grid that comprises 7.5 billion cells.

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Predictive digital twins
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AUTONOMOUS TRAJECTORY GENERATION AND CONTROL OF WELDING ROBOT MANIPULATOR FOR TUBULAR WORKPIECES USING DIGITAL TWIN

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ABSTRACT

Industrial robots are undergoing rapid evolution within the manufacturing sector. Two primary methods for programming robots include online programming via pendants and offline programming. However, employing the conventional online teaching method via the robot teach pendant for programming industrial robots is a laborious and time-consuming process that demands skilled expertise and disruption of the production line. A digital twin serves as a virtual representation of a physical object and process. This study aims to utilize a digital twin to facilitate offline autonomous welding path generation and advanced autonomous control of KUKA 6 Degree of Freedom (DOF) industrial welding robot manipulator for various tubular workpieces within the ROS environment and Python programming. The system's architecture incorporates sensors' data input, 3D models, model reduction, end effector trajectory generation and robot control. The publishing component of the digital asset enables individual joint motion controls of the robot to maneuver the end effector to the optimal position and orientation relative to the workpiece. A welding operation is simulated to illustrate the data exchange between the robot within its workspace and its digital version. The acquired data is stored and manipulated to establish a base for generating optimal welding trajectories for tubular workpieces. For the most effective and reliable welding application on tubular workpieces, detailed dimensional information along the generated end effector trajectory is essential. The point cloud models of tubular specimens are generated through 3D scanning. The MIG welding torch path planning is derived from the 3D model of the workpiece and instrumented workpiece positioner system. The point cloud model of the tubular workpiece is simplified to a skeletal line to reduce model complexity. Furthermore, to enhance welding quality, cross-sectional shapes and dimensions of the workpiece are autonomously identified along the generated welding torch path using the 3D model and a shape signature algorithm. Subsequently, specific welding tasks are applied to each segment of the workpiece based on autonomously identified cross-sectional dimensions, shape types and generated trajectory.

Key words: Digital Twin, Model Reduction, 6 DOF robot, Autonomous Trajectory Plannin

16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics

July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PROXIMAL GALERKIN: A STRUCTURE-PRESERVING FINITE ELEMENT METHOD FOR POINTWISE BOUND CONSTRAINTS

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[2]*Simula Research Laboratory*

ABSTRACT

The proximal Galerkin finite element method is a high-order, low iteration complexity, nonlinear numerical method for solving variational inequalities that arise from pointwise bound constraints in infinite-dimensional function spaces. This talk will introduce the proximal Galerkin method and demonstrate how it preserves the geometric and algebraic structure of pointwise bound constraints, leading to robust, mesh-independent algorithmic solutions to solve free boundary and optimal design problems. This talk is based in part on [1] but will include new results and applications.

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Certification of simulations and model adaptation in computational science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADAPTIVE IMPORTANCE SAMPLING FOR OPTIMIZATION WITH THE CONDITIONAL VALUE-AT-RISK

Brendan Keith[*1], Boyan Lazarov[2], Anton Malandii[3] and Stanislav Uryasev[3]*

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[2]*Lawrence Livermore National Laboratory*
[3]*Stony Brook University*

ABSTRACT

Engineering design involves estimating and optimizing immediate and long-term performance, manufacturing and maintenance costs, system response, levels of damage, and numerous other quantities of interest. In such environments, practical decisions are regularly made with significant aleatoric uncertainty, incomplete system knowledge, and various physical or financial constraints. In order to characterize a safe, reliable, and cost-effective product, a careful assessment of risk must be incorporated into the decision-making process.

Low-probability, high-consequence events can be mitigated by specifying a target quantile and optimizing for the associated tail expectation, also known as the conditional value-at-risk (CVaR) [1]. However, most techniques for CVaR optimization become prohibitively expensive for large quantiles because of the low frequency of drawing samples in the tail. In this talk, we present an efficient stochastic algorithm for CVaR optimization where the sampling distribution is adapted at every iteration to increase the probability of drawing samples in the tail. In turn, an optimal sampling distribution is found hand-in-hand with an optimal design variable. We use various design problems in engineering, particularly topology optimization under uncertainty, to illustrate the approach.

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IMPROVING ALGEBRAIC MULTIGRID PERFORMANCE FOR HIGH-ORDER FINITE ELEMENTS WITH MULTIPOINT CONSTRAINTS

Máté Kelemen[*1], Roland Wüchner[1] and Suneth Warnakulasuriya[1]*

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ABSTRACT

The main goal of high-fidelity structural analyses is recovering a detailed stress field, which makes high-order element formulations particularly appealing. In an effort to reduce the complexity of large assemblies, multipoint constraints are often used to represent subcomponents. Since these large problems are too big for direct solvers, they are usually solved with iterative algebraic multigrid solvers [1]. However, traditional AMG (algebraic multigrid) solvers are ill-equipped to handle linear systems produced by high-order finite elements efficiently. An option to improve their performance is exploiting the high-order formulations to perform optimal coarsening on the first few levels [2, 3]. Nevertheless, such methods have limitations, such as failing to handle multipoint constraints.

In this work, we extend the hybrid geometric-algebraic multigrid linear solver with support for multipoint constraints. Benchmark cases comparing the performance of existing methods to the proposed one are studied.

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Modeling and simulation of advanced manufacturing processes for metals
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A CRYSTAL PLASTICITY MODEL TO STUDY STRESS LOCALIZATION AND SIZE-DEPENDENT TENSILE PROPERTIES OF ADDITIVELY MANUFACTURED NICKLE-BASE SUPERALLOY: HAYNES 214™ AT ELEVATED TEMPERATURE

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ABSTRACT

Microstructures found in additively manufactured (AM) components often display unique characteristics in contrast to those produced using conventional manufacturing processes. Generally, these differences stem from the specific thermal histories experienced at the local level during the additive manufacturing build process. Previous research has illustrated that the mechanical properties of AM thin-walled structures (TWSs) can experience significant variations in response to changes in wall thickness, and this variability is dependent on temperature. The impact of temperature on these variations becomes more pronounced, particularly at elevated temperatures. The goal of this research is to investigate the nature of this size effect on tensile properties, such as yield strength, strain hardening rate, and ductility, for AM HAYNES 214 particularly under conditions of elevated temperature. To explore the size effect, thin-wall structures were fabricated with four different thicknesses: 1.0mm, 1.5mm, 2mm, and 2.5mm. To obtain the constitutive response, initially, we developed a robust approach to generate a representative volume element. Commencing with electron backscattered diffraction (EBSD) images of sections, the technique generates distributions of various morphological and crystallographic parameters, such as grain sizes, texture, and twin fraction. The effectiveness of the entire methodology is confirmed through a successful comparison of different statistics derived from the simulated microstructures with the actual EBSD data. Subsequently, we employed the Crystal Plasticity Fast Fourier Transform (CPFFT) based spectral method and relying on the phenomenological hardening law. We have successfully established a correlation between the local stress analysis conducted at the grain level and the global mechanical behavior observed in experimental results. This comprehensive examination of stress and strain at the micro level has uncovered variations in mechanical properties that are directly linked to the thickness of the TWS. Additionally, we explored how the local stress state, influenced by grain neighborhood effects, contributes to the observed localization behavior. Variations in the arrangement and properties of neighboring grains can lead to different stress distributions at the micro level. We explored the factors that drive the non-uniform distribution of mechanical responses within the HAYNES 214 by addressing how the local stress state, influenced by these grain neighborhood effects, contributes to localization behavior. The manufacturing-induced plastic anisotropy in grain distribution discovered through this study opens avenues for future research. Specifically, it provides opportunities to modify the microstructural grain topology and solidification parameters, thereby influencing not only the mechanical behavior of TWs but also that of other load-bearing critical structures across various applications.

Advanced numerical techniques for fluid flow in porous media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A TWO-SCALE PHASE-FIELD MODEL FOR TWO-PHASE FLOW IN POROUS MEDIA

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ABSTRACT

Two-Phase flow in porous media is relevant for many applications and accurately capturing interfacial effects in an effective model is central to its modeling. The flow morphology can vary significantly for different physical settings and impact the behaviour on the macro scale. In order to better capture the effects of microscopic interface behaviour on the larger scale, we determine effective parameters from pore-scale information instead of relying on relative permeability curves. We use phase-fields to model two-phase flow on the pore scale with an advective Allen-Cahn formulation coupled to a Navier-Stokes equation. Using periodic homogenization we arrive at macroscopic equations and microscopic cell-problems that yield effective parameters [1]. Through numerical experiments we investigate the effects of saturations and pore-scale fluid morphologies on the computed tensors and the coupled two-scale simulation. We implement our phase-field model for two-phase flow in DuMux, using a finite volume discretization. It features staggered control volumes and a combination of cell- and facecentered variables, which communicate using a multidomain coupling manager. This serves as a solver for cell-problems in the two-scale formulation that results from upscaling. The coupling between scales is achieved using preCICE and the associated Micro Manager [2].

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A BAYESIAN NEURAL NETWORK APPROACH TO MULTI-FIDELITY SURROGATE MODELING

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ABSTRACT

This talk deals with the surrogate modeling of computer code results that can be evaluated at different levels of accuracy and computational cost, called multi-fidelity. We propose a method combining Gaussian process (GP) regression on low-fidelity data and a Bayesian neural network (BNN) on high-fidelity data, see [1]. The novelty, compared with the state of the art, is that uncertainties are taken into account at all fidelity levels. The prediction uncertainty of the low-fidelity level is transmitted by Gauss-Hermite quadrature to the high-fidelity level. In addition, this method takes into account non-nested designs of experiment and non-linear interactions between levels. The proposed approach is then compared to several multi-fidelity GP regression methods on analytic functions and on a mechanical computer code.

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Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMPROVED RELOCALIZATION USING REGULARIZATION IN COMPUTATIONAL HOMOGENIZATION OF COMPOSITE STRUCTURE

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ABSTRACT

Carrying out a Direct Numerical Simulation (DNS) of a heterogeneous structure seems expensive in terms of computational time and generally infeasible due to the high dimension of the system to be solved. The application of homogenization methods such as asymptotic homogenization [1], used in multiscale analysis of heterogeneous structures, allows not only a reasonable computational time but also a good efficiency. However, obtaining the local fields by straigthforward techniques like linear relocalization can induce discontinuties accross macro elements boundaries and low accuracy in presence of microstructure and strain gradients

We propose a novel approximation to estimate local fields in heterogeneous structures exhibiting a mesostructure gradient in the context of non scales separation. It improves the relocalization step by ensuring the continuity of the relocalized fields within a finite element framework for linear elastic heterogeneous materials.

The methodology involves the following steps. First, the structure is divided into non-periodic sub-domains. For each of these, a classical first-order homogenization is performed and the effective properties associated with that subdomain are calculated. A first spatial regularization of the effective properties is then performed on the structure. The macro problem is then solved using these macro effective properties. The resulting macro-deformations are regularized and used to perform a differential Kruch relocation process [2].

As a result, spurious discontinuities across macro-elements are reduced and the effects of deformation gradients can be captured even when using a first-gradient homogenization scheme.

Applications to composites or heterogeneous materials with microstructure gradients are presented to demonstrate the potential of the technique.

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Quantum scientific computing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPING A FORMULATION OF STRUCTURAL DESIGN OPTIMIZATION PROBLEMS FOR QUANTUM ANNEALING

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ABSTRACT

We develop a formulation of structural design optimization problems, which aims to be solved by quantum annealing (QA) on currently available devices. In structural design optimization, the goal is to improve the performance and efficiency of structures by finding the best design, e.g., a choice of component dimensions, that meets specific criteria, such as maximizing strength. This process typically involves computational optimization methods to explore various design possibilities. Here, a recently evolving strategy based on quantum mechanical effects is QA. In this context, a suitable problem needs to be provided in a specific formulation, e.g., as a quadratic unconstrained binary optimization (QUBO) model. Therefore, we present a corresponding formulation for structural design optimization problems. In such a problem, an analysis model is required to evaluate the structure's performance. For this purpose, we use energy minimization principles to determine how a structure behaves under applied loads. This allows us to merge the analysis problem with the optimization problem as one overall minimization problem. Finally, mapping this problem to a QUBO problem enables us to solve it with QA.

We apply this approach to a one-dimensional sizing problem of a compound bar under self-weight loading [1]. In this course, we study how specific aspects of the formulation influence the number of required qubits. The accuracy of the obtained results is evaluated by means of analytic solutions. In conclusion, we show that the presented formulation can be used to solve structural design optimization problems by QA on existing hardware.

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Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA DRIVEN AND HIGH FIDELITY MODELING APPROACHES TO ADVANCE UNDERSTANDING AND TRL LEVEL OF 3D PRINTING

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ABSTRACT

A multi-scale ALE3D high fidelity model is developed to simulate directed energy deposition additive manufacturing. The model aims at capturing at a high fidelity the powder transport from the coaxial nozzle to the work piece as well as the effect of the carrier gas and laser ray tracing heating and reveals a new kind of air-cushioned or shell-like pores as well as the advantages of ring laser beam profile. The high cost of modeling is brought down by using deep learning and data driven reduced order modeling at different scales. The end goal is to combine modeling with a data driven approach for “first time right” also referred to here as intelligent feedforward (IFF). We showcase how IFF is used to optimize laser power and scan speed to print complex large parts with overhang geometries, such as the Menger sponge, and obtain high geometric accuracy.

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FAST MULTIPLE SCATTERING ANALYSES IN REDUCED SPATIAL DIMENSIONS

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ABSTRACT

Volume discretization methods face multiple challenges when used for exterior scattering analyses including high computational cost, need for artificial domain truncation and accurate boundary representation. These challenges are more pronounced in multiple scattering analyses where the wave moves back and forth between multiple obstacles. Conventionally such problems are solved by meshing the space between obstacles and truncating the domain with a fictitious boundary enclosing them. This makes mesh generation even more challenging and considerably limits the flexibility to move, rotate, and reshape the scatterers which are required for design and optimization of devices relying on wave propagation phenomena. Hence, spatial dimension reduction is highly desirable. Methods relying on boundary integral equations allow spatial dimension reduction, however, these methods introduce new challenges such as the need to treat singular integral kernels and lead to dense and possibly ill-conditioned matrices limiting them to low- to mid-frequency analyses. Like boundary integral methods, On Surface Radiation Conditions (OSRC) require boundary discretization only and lead to integral equations with smooth kernels. We demonstrate possibility of enhancing the accuracy OSRC for single and multiple scattering analyses and adopt it to develop a well-conditioned method based on fundamental solution. These developments [1, 2] reduce the spatial dimensions by one as the interaction between scatterers are captured analytically; the need for treating singularities is eliminated; and reliable single and multiple scattering analyses can be performed for arbitrarily shaped scatteres in mid- to high-frequency regimes.

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Trustworthy multi-fidelity and data-driven models for computational applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ACCELERATING MANUFACTURING PROCESS DISCOVERY IN MATERIAL SCIENCE THROUGH MULTI-FIDELITY NEURAL NETWORKS

Mohammad Khalil[*1], Ankit Shrivastava[1], Matias Kalaswad[1], Habib Najm[1] and David Adams[1]*

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ABSTRACT

Machine learning (ML) is gaining popularity in material sciences to facilitate the optimization of manufacturing processes that deliver materials with desired properties. In such settings, the limited availability of high-fidelity data (e.g. from costly simulations/experiments) is compounded by the need for high-capacity ML models to capture complex underlying physics. When available, lower-fidelity datasets can be exploited to enhance the predictive accuracy of ML models. In this presentation, we will present a recently developed bi-fidelity neural network training strategy that combines low-fidelity synthetic data with costly high-fidelity experimental data to predict high-dimensional quantities of interest. Specifically, we are interested in predicting the crystallographic texture of molybdenum coatings across a range of process conditions. The bi-fidelity neural networks are trained to capture high-dimensional X-ray diffractograms via low-dimensional latent variables obtained through principal component analysis, exhibiting enhanced predictive accuracy in comparison to traditional learning using limited volume of high-fidelity data.

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A TERZAGHI BASED APPROACH TO CONSOLIDATION ANALYSIS OF UNSATURATED SOILS

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ABSTRACT

In this work, a framework is presented for the determination of pore pressures dissipation and settlement calculations during the one-dimensional consolidation in unsaturated soils. To this end, two independent diffusion-form partial differential equations similar to Terzaghi's consolidation equation are presented. Modified coefficients of consolidation for water and air phases are introduced to capture the transient flow of water and air phases during consolidation. The coefficients of consolidation are determined according to the initial state of the unsaturated soil. The solutions to these partial differential equations yield the pore water and pore air pressures at any depth and at any time in the soil layer during consolidation. A set of dimensionless curves analogous to those proposed by Terzaghi are presented to illustrate the pore water and pore air distribution during the consolidation of unsaturated porous media, permitting hand calculation of the consolidation process. The validity of the approach is demonstrated through comparison with fully coupled numerical analysis of the problem. The excellent agreement is obtained between hand calculations and the numerical results.

Next-generation numerical methods for coupled multiphysics problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

UNVEILING OPTIMAL CONTROL OF DOUBLY DIFFUSIVE FLOWS: NEW INSIGHTS FROM THEORY AND NUMERICAL ADVANCEMENTS

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ABSTRACT

This talk dives into the exciting world of optimal control of doubly diffusive flows, exploring recent theoretical advances and numerical breakthroughs. We'll unveil minimal regularity results for the governing equations, groundbreaking for their relevance beyond this specific field. Next, we'll delve into the $H^{\textrm{div}}$-conforming discontinuous Galerkin formulation, a powerful method for tackling these complex flows. Moreover, we'll establish the efficiency and reliability of residual-based a posteriori error estimators, ensuring accurate solutions at every step. Finally, we'll put these tools to the test, simulating the captivating phenomenon of small particle sedimentation in salinity-driven flows. Witness numerical results that not only validate our theoretical claims but also showcase the power of adaptive solution algorithms guided by our innovative error estimators.

Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CFD MODELLING OF ARTIFICIAL PLUME DYNAMICS FOR REEF CONSERVATION: UNVEILING BENCHMARKS FOR LARGE-SCALE IMPACT

Saima Bukhat Khan[*1], Joel Alroe[1] and Emilie Sauret[1]*

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ABSTRACT

Solar shading through the artificial production of marine fog is an innovative technique to mitigate the impacts of climate change on coral reefs. This process uses more than a thousand nozzles arranged in parallel to atomise sea water. The plume formed from the primary and secondary breakup of the sea water droplets extends over distances of more than 1km, creating a plume that scatters sunlight and shades the reef. To precisely evaluate the quality and extent of the plume to protect the reef, the accurate estimation of the plume characteristics are critical. This, however, depends on the atomisation process to generate minuscule droplets. Computational Fluid Dynamics can become a powerful tool to simulate such multiscale problems.

Past models have tackled urban haze and fire plumes using Computational Fluid Dynamics (CFD) and do not require any length precisions. Artificial plumes which are made from sea water requires precise length for fogging and shading purposes. The breakup of particles contributes to the formation of smaller droplets which are essential for plume formation. While CFD adeptly models the atomisation phenomena of single and multiple nozzles, analysing larger-scale problems remains unexplored.

The purpose of this study is to establish a benchmark for large scale scenarios involving arrays of nozzles. The physical setup consists of 1080 nozzles arranged in parallel with each fogging nozzle manifold of 12 nozzle lines and 15 nozzles per line for 6 nozzle arrays. Each nozzle has orifice diameter of 200 micrometres and nozzle array has dimensions of around 1626mm by 1270mm. The model is divided into two steps: spray breakup using single and multiple (four) nozzles with and without impaction pin configuration and its dispersion in air flow using nozzle array framework. The spray breakup step describes the subsequent breakup of droplets to the position where droplet velocity equals air velocity. This step will help in getting deeper insight into downstream flow. Nozzle spray dimensions and droplet trajectory analysis will provide the boundary conditions for the second step of nozzle array for large scale modelling. Overall, this study presents a systematic evaluation of Lagrangian-Eulerian approach to create a benchmark case for large scale plume modelling using sea water spray with single and multiple nozzle configuration. The evaluation is based on grid-sensitivity analysis with focus on impact of turbulence model for continuous phase (air), the number of particle streams for discrete phase (sea water) and nozzle spray angle.

Innovations in machine learning-enhanced uncertainty quantification for computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

QUANTIFICATION OF FABRICATION-RELATED UNCERTAINTIES IN TPMS LATTICES WITH IMAGE PROCESSING AND SURROGATE MODELING

Waris Khan[*1], Ece Naz Erulker[2], Gullu Kiziltas[2] and Pinar Acar[1]*

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ABSTRACT

This paper addresses the quantification of fabrication-related uncertainties in Polydimethylsiloxane (PDMS) Triply Periodic Minimal Surface (TPMS) lattice structures using image processing techniques and surrogate modeling. The aim is to develop a Finite Element (FE) model that captures the uncertainties originating from thermal and mechanical fluctuations during the 3-D printing process, enabling the assessment of homogenized mechanical properties crucial for various engineering applications.

The fabrication process often introduces deviations in TPMS lattices such as defects and surface distortions. To quantify these variations, micro-computed tomography (micro-CT) imaging is employed, providing cross-sectional images of the PDMS lattice morphology produced using 3D printed sacrificial molds. Image processing algorithms are then applied to parametrically quantify deviations, laying the groundwork for subsequent analysis.

Next, the image-based data is incorporated into a sophisticated FE model, allowing for a realistic representation of the TPMS structure's mechanical behavior. To validate the prediction accuracy of the FE model, its results for stress and strain fields are compared to the experimental data. Remarkably, a close match is observed between the experimental data and the FE model predictions, affirming the effectiveness of our approach in capturing the intricate interplay of fabrication-related uncertainties. This agreement not only validates the accuracy of the FE model but also underscores the significance of our image-processing methodology in quantifying fabrication-related uncertainties.

Furthermore, we develop a neural network (NN)-based surrogate model to predict the homogenized mechanical properties as a function of the parametric representation of the TPMS lattice structure obtained through image processing. This surrogate model improves the computing times required for the determination of mechanical properties and thus allows for the efficient creation of sufficient statistical data needed for assessing the propagation of the uncertainty on properties. Accordingly, the surrogate model representation is utilized to predict the effects of uncertainty on the homogenized mechanical properties as a function of the variations in the geometric parameters of the TPMS lattices resulting from the fabrication-related uncertainty.

In conclusion, present study contributes to a deeper understanding of lattice behavior under real-world fabrication conditions, advancing the design and application of TPMS lattices in various engineering fields. The study's findings are expected to enhance the reliability and performance of TPMS lattice structures in applications such as lightweight structural components and biomedical scaffolds.

Advances in computational mechanics for flow-induced vibrations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A HYBRID MODEL FOR FLOW-INDUCED VIBRATIONS OF PIPES CONVEYING FLUID SUBJECTED TO EXTERNAL CROSS FLOW

Mahdi Riazat[1], Mojtaba Kheiri[1], Brian Vermeire[1] and Weixing Yuan[2]*

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ABSTRACT

We present a hybrid analytical-computational model for studying the flow-induced vibration (FIV) of a pipe conveying fluid subjected to an external cross flow. Real-world cylindrical structures subjected to fluid flow (e.g., drilling risers and seawater intake risers) are often arranged such that combined loading with complex interactions between different FIV modes appears. These interactions often result in unexpected, unsafe dynamical behaviour, such as chaotic motions, and amplified amplitude of vibrations. Several attempts have been made so far to study these interactions for drill- and brine-string systems. Dynamics and stability of long pipes conveying fluid, simultaneously subjected to external cross flow were studied by several researchers, such as Dai et al. [1]. They found that self-excited vibration (SEV) and vortex-induced vibration (VIV) caused by axial and cross flows, respectively, may weaken or amplify each other, and that the system may display complex dynamical behaviour, such as inverse period-doubling bifurcations and chaotic motions. All those studies, however, adopted analytical models for examining the stability and dynamics of the system. Although analytical models for SEV of pipes conveying fluid are well-established in the research community, studies have shown that analytical models, such as the wake oscillator model, used for modelling VIV, still need considerable improvement. In this study, we develop a novel model by combining a three-dimensional nonlinear analytical model for SEV of pipes conveying fluid [2] with a computational fluid dynamics (CFD) model for VIV due to external cross flow [3]. This hybrid model obviates the need for a fully computational model where both internal and external flows are solved using CFD, thus significantly simplifying the modelling and reducing the computational time. The numerical results are presented for two configurations: a pipe conveying fluid immersed in a stationary fluid, and a pipe conveying fluid subjected to an external cross flow.

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Imaging and computational methods for biomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL MODELING OF THE RODENT HEART AND ITS RESPONSE TO PRESSURE OVERLOAD

Vitaly Kheyfets[*1], Ilham Essafri[1], Mengqian Zhang[1], Ella Lyon[21], Kurt Stenmark[1], Kenzo Ichimura[3] and Edda Spiekerkoetter[3]*

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ABSTRACT

When the human heart is subjected to pressure overload, it responds to the elevated mechanical stress with a complex concert of changing gene expression, remodeled coronary microvasculature, and altered cardiac tissue structure. This also leads to a disruption of mechanical energy transfer between the left (LV) and right ventricles (RV), which has a profound effect on pumping function. The overall objective of our work is to pair a multi-scale computational model of a rodent heart with ongoing experiments to bridge the gap between transcriptomics, non-Newtonian fluid dynamics in the coronary microvasculature, and changes in tissue structure. This would allow us to identify which aspects of remodeling are beneficial to cardiac pumping function and myocardial nutrient supply, and possibly isolate targets for intervention.

We performed catheterization, cardiac MRI, and deep tissue imaging on 8 healthy rodents and 8 subjected to 7 weeks of chronic RV pressure overload. This data was combined to develop a 0-dimensional (0-D) digital twin of the heart and pulmonary circulation, by optimization, to fully characterize cardiac function and pulmonary arterial impedance. The optimized 0-D model is applied as a boundary condition to a rodent specific 3D finite element model (FEM) of the heart, with contractile mechanics optimized to regional tissue strain (measured by feature tracking applied to cardiac MRI images). Finally, deep tissue images of biopsied heart tissue were used to develop 3-D networks of the coronary microcirculation, which were used for non-Newtonian computational fluid dynamics simulations.

We developed a novel approach for sensitivity and practical identifiability analysis by combining supervised machine learning with game theory, which revealed a subset of identifiable rodent-specific 0-D modeling parameters. Ongoing FEM modeling has revealed that changes to the RV microstructure to a certain degree improve RV pumping function, but at the expense of LV-to-RV mechanical coupling. CFD models of the 3D microvascular network showed that capillary remodeling reduces hemodynamic stress and likely serves to preserve nutrient delivery to the surrounding tissue by maintaining a low capillary resistance.

Leveraging in-silico modeling to study how the rodent responds to pressure overload has yielded invaluable insight into multiple aspects of this response, which were previously inaccessible through conventional experimental approaches. Combining these findings with ongoing bioinformatics analysis offers a promising avenue for bridging the gap between mechanical stress, gene expression, and structural response. Ultimately, when applied to the human, we hope for this technology to project pathways of restoring function by model prediction.

Current trends and advances in enriched finite element methods and coupled simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING THE ENHANCED GEOTHERMAL SYSTEMS USING THE EXTENDED–FEM AND AN EQUIVALENT CONTINUUM MODEL

Amir R. Khoei[*1], S.M.S. Mortazavi[1], O. Rezaie Beydokhti[1] and P. Pirmoradi[1]*

[1]*Sharif University of Technology*

ABSTRACT

In this paper, a computational technique is presented for Thermo-Hydro-Mechanical (THM) simulation of Enhanced Geothermal Systems (EGS) based on the local thermal non-equilibrium using the eXtended Finite Element Method (XFEM) and Equivalent Continuum Method (ECM). Heat extraction from Enhanced Geothermal Systems involves several multi-physics coupling processes, including the seepage through the fractured porous media, the thermal exchange between the working fluid and the matrix, and the deformation of fractured porous media, which play essential roles in exploiting the geothermal energy contained in hot dry rocks. The ECM can provide the equivalent tensors of not only fluid permeability but also solid compliance, which is an essential feature for coupled Thermo-Hydro-Mechanical simulation of fracture networks. In the model, the XFEM is employed for large-scale fractures to capture the mass and heat transfer between the fracture and matrix more accurately, while the ECM is applied on the network of small-scale fractures since considering their details explicitly is not usually cost-effective. Hence, the proposed model benefits from the advantages of both methods, and it allows for managing between accuracy and cost. The set of THM equations is solved with both Local Thermal Equilibrium (LTE) and Local Thermal Non-Equilibrium (LTNE) assumptions to find out the impact of each method on the production temperature.

The model is validated against the analytical solutions of heat transfer in porous media as well as single fracture problems. Moreover, its flexibility and applicability are shown by assessing the effects of the connectivity of fractures, characteristics of fracture networks, coupling conditions, and local thermal non-equilibrium assumption on the EGS simulation results. It is observed that the network connectivity and fracture alignment are both influential in the early thermal breakthrough; however, each can take dominance under different conditions. The capability of the proposed computational model is demonstrated for the diagonal arrangement of the injection and production wells with different fracture orientations in-between. The simultaneous effects of fracture connectivity and inclination are investigated between the two injection and production wells. It is observed that the temperature difference between the two cases is higher in the middle of the domain by comparing the results of LTE and LTNE assumptions. Moreover, it is concluded that the LTE model overestimates the fluid temperature in comparison to the LTNE model in cold water injection problems. The results show the proposed computational model is a promising tool for estimation of the heat mining performance of EGS.

Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATION OF PARTIAL NODAL STRAIN SMOOTHING IN ENHANCING THE ACCURACY OF THE LINEAR FINITE ELEMENT METHOD FOR COUPLED PROBLEMS OF GEOMECHANICS

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ABSTRACT

In this study, partial nodal strain smoothing is incorporated into the framework of the linear finite element method to develop a novel numerical technique, referred to as partial node-based smoothed FEM (PNS-FEM), for flow-deformation analysis of problems in geomechanics. In the PNS-FEM, the stiffness and permeability matrices of the domain are computed using the formulation of the linear FEM enhanced with partial nodal strain smoothing. The PNS-FEM takes advantage of the contradicting errors inherent in the solutions of the linear FEM and the node-based smooth point interpolation method (NSPIM) to yield close-to-exact solutions. The formulation of the PNS-FEM and the steps required to develop a PNS-FEM code from an FEM code are presented. The performance of the PNS-FEM is then examined through several numerical examples encompassing both linear and nonlinear porous materials subjected to various loading conditions. The results show that partial nodal smoothing is a simple and effective technique to considerably improve the performance of the linear FEM in coupled problems of geomechanics.

Geomechanics of the cryosphere
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREDICTING SEA ICE BEHAVIOR AND STRESS-STRAIN CHARACTERISTICS: A DATA-DRIVEN APPROACH

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ABSTRACT

The Arctic Sea ice cover is undergoing a profound transformation in response to climate change, leading to a future ocean with open waters in summer and only annual ice in winter similar to the Antarctic. This shifting landscape presents both opportunities and challenges, particularly for offshore infrastructure development. As the Arctic opens up to resource extraction, shipping, and commercial activities, the need for resilient infrastructure that can withstand the unique forces of sea ice becomes increasingly crucial. Sea ice exhibits complex mechanical behavior, with ductile and brittle modes of failure under compression. Capturing these distinct stress-strain signatures and failure mechanisms is critical for predicting ice forces on structures. To address this challenge, this study delves into the intricate mechanics of sea ice behavior, employing data-driven techniques to enhance the understanding and design capabilities. comprehensive stress-strain databases were compiled from sea ice compression tests conducted under various conditions, representing the diverse characteristics of Arctic Sea ice. The databases served as the foundation for developing machine learning models, including deep neural networks and decision trees, capable of distinguishing between ductile and brittle sea ice behavior. These models also predicted peak and residual stress-strain, providing valuable insights into the mechanical properties of sea ice. To gain deeper insights into the factors driving sea ice behavior, an analysis of model variable importance was conducted. This analysis revealed the key parameters that significantly influence sea ice strength and deformation characteristics under varied conditions. The results highlighted the impact of strain rate, grain size, temperature, and peak and residual stress and strain values and sea ice behavior. The developed predictive models and the insights gained from variable importance analysis demonstrate the power of data-driven techniques in advancing sea ice constitutive modeling. These advancements are essential for the design of robust offshore infrastructure that can withstand the dynamic and unpredictable forces of sea ice in the evolving Arctic. As climate change reshapes the Arctic landscape, data-driven approaches will play a pivotal role in enabling safe and sustainable development in this challenging yet promising region.

Methods for identification, machine learning, and uncertainty quantification of reduced order models of coupled systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VARIATIONAL INFERENCE FOR A STOCHASTIC MULTICLOUD MODEL

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ABSTRACT

In the backdrop of climate change the evolving weather and climate is posing a challenge to the numerical modellers to predict the observed variability in a realistic manner. The bottleneck in this endeavour is the improper representation of clouds and its feedback to the environment in climate models. The first author and collaborators have proposed in the recent years a stochastic modeling framework to represent the sub-grid variability, in climate models, associated with clouds and organized convection in the tropics. The model is based on a lattice interacting system that mimics the dynamical transitions of coldness between several cloud types as revealed by satellite and radar observations, in the form of a Markov process with transition probabilities that depend on some physical variables via a set of transition time scale parameters than are indirectly learned from radar data, using Bayesian inference. However, due to the model's complexity, the likelihood function is not known in closed form and depends on the solution of the Kolmogorov backward equations which amount to computing an exponential matrix of high dimension (~10^6). To overcome this computational challenge a variational inference algorithm has been adopted for the learning problem and its efficacy and efficiency have been tested in the context of an AR1 model where various blackbox algorithms used in neural network studies have been tested and validated.

PSE (Problem Solving Environment)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPOSABLE HPC INFRASTRUCTURE FOR CONTINUUM MECHANICS AND AI WORKLOADS

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ABSTRACT

High-performance computing (HPC) applications like computational fluid dynamics are often compute intensive, but not all scientists have access to such powerful supercomputers. Cloud computing is a viable alternative for running these applications on the cloud without needing large capital expenditure (CAPEX) in high-end parallel computing systems. However, transitioning from a managed supercomputer to a self serviced public cloud is not straightforward for researchers from engineering disciplines. Moreover, the novice user lacks a priori knowledge of performance for continuum applications on cloud. This preparatory phase can sometimes be rather expensive due to unpredictable costs of cloud computing. The aim of this paper is to provide guidelines for running typical continuum mechanics and AI workflows on HPC clusters in the public cloud. The selected use cases are: CFD, CSM, EM, atmospheric science, geoscience and deep learning training and inference. We will also provide the performance comparison of public cloud and supercomputer for all benchmarks selected from a wide range of applications at various spatial/temporal resolutions. We hope to provide guidelines to individual researchers, faculty groups, academic departments and SMEs for selecting specifications for their respective workloads. These specifications include: compute instances (CPUs/GPUs), storage, interconnect, RAM, scheduler, software environment and data management. We believe that unbiased reporting of HPC workloads on cloud is essential for policy makers for making long term planning for HPC infrastructure. A cloud alternative to a managed on-premise supercomputer provides an option to convert capital expenditure to operational expenditure.

Keywords: Continuum Mechanics, HPC, On-demand Infrastructure, Artificial Intelligence

Multiscale computational and data-driven approach of advanced materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE STUDY ON THE THERMAL CONDUCTIVITY OF VITRIMER-BNNT NANOCOMPOSITE.

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ABSTRACT

With the help of advanced manufacturing and characterization technique in the field of engineering materials, there have been continuous attempts to replace traditional metal or ceramic materials with high performance polymers and composites in various applications. The notable advantage of polymer's durability such as cross-linked thermosets, however, paradoxically leads to non-degradability and eco-friendly issues. The limited recycling of plastic waste reaching approximately 10% naturally sparked interest in lightweight composites that can secure higher recyclability, less toxicity while maintaining excellent mechanical and thermal properties.

Vitrimer is a polymer featuring dynamic and reversible crosslinks between atoms that allow for recyclability while maintaining good physical properties, representing a recyclable alternative. Above all, the vitrimer's distinguishing feature lies in dynamic crosslinking, activated under specific conditions such as heat or light, providing control between polymer chains. Therefore, understanding the vitrimer's stimuli responsive cross link mechanism is of primary concerns for its application.

BNNT(boron nitride nanotube) is a low dimensional tubular structure comprising alternating boron and nitrogen, The BNNT exhibits mechanical and thermal properties comparable to the CNT, along with piezoelectricity, exceptional thermal stability and cytocompatibility. However, experimental research is hampered by its high cost reaching approximately 80 dollars per gram for controlled synthesis with high-purity. Overcoming these challenges necessitates an in-silico simulation study and sequential multiscale modeling approach for the vitrimer/BNNT nanocomposites.

This study demonstrates a sequential multiscale modeling approach for thermal transport properties of virtrimer/BNNT nanocomposites combining classical molecular dynamics simulations and composites micromechanics models. The dynamic cross linking of vitrimer is described using a bond-boosting method and the resultant thermal conductivity of the vitrimer is determined according to the switching of cross links. Interfacial thermal conductance between the BNNT and vitrimer is investigated through a laminated interface model to quantify the phonon scattering and Kapitza thermal resistance. To develop an efficient structure-property relationship model, the constitutive model for thermal conduction of nanocomposites with interphase and Kapitza resistance is derived from the multi-inclusion model with an equivalent filler concept to describe the degradation by the phonon scattering. Finally the vibrational density of state and solubility parameters of vitrimer with varying dynamic cross link density and BNNT were discussed to correlate the process-structure relationships.

This work was supported by KOREA HYDRO & NUCLEAR POWER CO., LTD (No. 23-Tech-04)

Modeling and simulation of the electro-chemo-thermo-mechanical interactions in energy transition and energy storage systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTATIONAL CHEMO-MECHANICS WITH APPLICATION TO MULTIFUNCTIONAL AND HIGH-TEMPERATURE MATERIALS

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ABSTRACT

This presentation gives an overview of our current research activities in the area of chemo-mechanics-based material modeling. Building on experience in theoretical and computational methods for multiphysics problems, our interest here lies in the modeling of nonlinear, dissipative material behavior in which interacting thermo-chemo-mechanical processes play a dominant role. We aim to capture mechanisms such as stress- and temperature-biased phase transitions and chemical reaction-diffusion processes that directly influence, or even enable, the effective behaviors of modern engineering materials. In this general multiscale approach, model formulations may be considered on very different length and time scales. Recent work regarding analytical and computational scale-bridging methods is also briefly discussed.

Three fundamental ingredients are addressed in this talk: (i) the theoretical model development, particularly regarding variational settings, (ii) the numerical treatment of these problems, and (iii) the calibration of thermodynamical properties via the CALPHAD method. Regarding the first aspect, we discuss the advantages and disadvantages of formulations for chemo-mechanical multifield problems through minimization and saddle-point principles. In terms of numerical solution schemes, we elaborate on the finite element implementation of such theoretical frameworks. Our particular approach builds on the flexible and quite general utilization of the UserELement interface (UEL) provided in the FE software package Abaqus. We further discuss ongoing collaborative work on the co-design of the variational model development and parallel solvers for chemo-mechanics problems, for which the MPI-parallel implementation instead is based on the software libraries deal.II, p4est and FROSch (Fast and Robust Overlapping Schwarz). Moreover, a concept is proposed in which thermodynamically informed material models are efficiently achieved via CALPHAD-trained neural networks. Representative numerical examples from a broad spectrum of technologically relevant studies — ranging from hydrogels to multifunctional filters for the cleaning of steel melts — are presented to demonstrate the validity and flexibility of our simulation frameworks.

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Machine learning for design tasks and inverse problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN MORPHOGENESIS WITH PERSISTENT HOMOLOGY FOR SOLVING TOPOLOGY OPTIMIZATION PROBLEMS

Taisei Kii[*1], Kentaro Yaji[1], Hiroshi Teramoto[2] and Kikuo Fujita[1]*

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ABSTRACT

Topology optimization is a powerful approach for realizing novel structural optimization by solving a material distribution problem under a high degree of design freedom. In exchange for this attractive feature, topology optimization cannot typically avoid multimodality caused by complex physical computational models, where multiple undesirable local optima exist.
Evolutionary algorithms (EAs), inspired by the emergent process of biological evolution, are capable of global solution search and are considered effective for optimization problems like the one mentioned above. However, the search performance of typical EAs is significantly degraded for large-scale problems, making it difficult to solve topology optimization problems.
Focusing on dimensionality reduction with deep generative models to address such challenges, this study proposes a framework based on the previous work [1], in which the design candidates are iteratively updated by a variational autoencoder (VAE). Furthermore, we apply effective crossover operation into the latent space of the VAE to incorporate the essence of EAs [2]. As a key component of the proposed framework in this study, we employ persistent homology to essentially maintain the diversity among structures represented as high-dimensional material distribution data. Persistent homology is one of the topological data analysis methods in which topological features such as the number of connected components and voids and their sizes are extracted from the target complex data into a two-dimensional plot called a persistent diagram. The Wasserstein distance between corresponding persistent diagrams quantifies the difference in topological features between material distribution data. We develop the proposed framework incorporating the selection operation based on the Wasserstein distance and name it data-driven morphogenesis as a new concept of the EA-based optimization method using a generative model.
We apply the proposed framework to topology optimization problems with strong multimodality. Firstly, we confirm the extraction of topological features of the structures using persistent homology. Next, we compare the obtained optimization results with those obtained by conventional topology optimization. The optimized structures improved by the proposed selection operation exhibit comparable or better performance than those by typical topology optimization, demonstrating the usefulness of data-driven morphogenesis for solving topology optimization problems.

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16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics

July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STRUCTURAL TOPOLOGY DESIGN FOR FUNCTIONAL MOTION AS WELL AS FUNCTIONAL MECHANICS

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ABSTRACT

Concept of topology optimization has been widely accepted to design mechanical functionality, heat transfer characterization, flow domain for fluid, and material properties. Details and widely spread advanced research results have been published in, e.g., Computer Methods in Applied Mechanics and Engineering.

In this talk, a new notion of topology optimization to generate dynamical motions of a possibly soft structure, will be presented by collaboration with Tsuyoshi Nomura Research Group in Toyota Central Research and Development Laboratories. This study shows an extension of the notion of topology optimization to motion related functional design of a structure that may be applicable to soft robot design, and motion creation of a living creature in gaming software.

Design and mechanics of mutifunctional composites and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ANALYSIS OF COMPOSITE STRUCTURAL LITHIUM-ION BATTERIES AND AN APPLICATION TO A DOOR STRUCTURE OF ELECTRIC VEHICLES

Cheol Kim[*1] and Yeongeun Park*[1]

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ABSTRACT

The structural lithium ion battery may serve the dual purpose of providing support for loads and storing electrical energy. A composite structural lithium ion battery, which incorporates carbon fibers and a semi-solid matrix exhibiting favorable electrical conductivity and hyper-elastic material behaviors, has been developed for a potential application to electric vehicles. The analysis in this study includes evaluations of mechanical, electrochemical, and crash performances, with optimization of design parameters for this innovative structural battery. A structural battery cell is the basic unit of a structural battery and consists of an anode, a cathode, an electrolyte, a separator, and a current collector. A separator layer is located between the anode and cathode. To prevent the structural battery laminate from warping, all layers are arranged symmetrically with respect to the center layer. Finite element analyses are performed on the RVE model to derive the mechanical properties of the composite lamina of structural battery. After constructing the door of an electric vehicle with a structural battery, a crash analysis is performed to check the crash performance of the structural battery. Parametric studies were conducted on 11 design variables, encompassing factors such as layer thickness, fiber angle, cathode coating thickness, and fiber volume fraction. Bayesian optimization was employed to maximize the electric vehicle range, ensuring compliance with specified mechanical properties. In this study, the effectiveness of structural batteries is demonstrated through one application case, an auxiliary power source for electric vehicles.

FEASIBILITY OF VEHICLE-BRIDGE INTERACTION NEURAL OPERATOR FOR DRIVE-BY BRIDGE DAMAGE DETECTION

Joshua Irawan[1] and Chul-Woo Kim[1]*

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ABSTRACT

Drive-by bridge damage detection using vehicle vibration has been actively studied in recent years, including machine learning-based approaches. However, extracting features related to the condition of bridges remains a challenge. With supervised learning methods, obtaining training data on a bridge's damage state is almost impossible. Unsupervised learning approaches, on the other hand, can only yield relative changes in features rather than physical characteristics related to structural performance. This study aims to propose and investigate the feasibility of a vehicle-bridge interaction neural operator (VINO) for bridge damage detection using vehicle vibrations. The VINO is first constructed using the physically informed training data from numerical simulations of vehicle-bridge interactions considering the damage field of the bridge. Then data-informed fine-tuning of the VINO is carried out using available data from the target bridge. It is noted that no damage data is required in the fine-tuning stage. The feasibility of VINO for drive-by bridge damage detection is discussed using an in-house experiment.

Recent advances in high-order methods for computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN SHOCK-CAPTURING INDICATOR FOR DISCONTINUOUS GALERKIN METHODS WITH DECISION TREE CLASSIFIERS

Dongseok Kim[*1], Jayeon Joo[1] and Chongam Kim[1]*

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ABSTRACT

Much efforts has been put on finite element-based high-order methods for scale-resolving compressible simulations, due to their capability to handle complex geometries with high-order accuracy and cost-efficiency. At the same time, high degree polynomial-based discretizations are susceptible to shock-driven instability, known as Gibbs oscillations. Typically, unphysical numerical oscillations near shock waves are handled by suitable shock-stabilization techniques, such as limiting strategy and artificial viscosity. Before applying any of these techniques, however, the occurrence and location of shock must be identified. Some troubled-cell indicators, such as P1-projected MLP condition [1] and troubled boundary detector [2], have been developed and successfully combined in a hierarchical projection manner. But the precise detection of troubled-cells is non-trivial and there is still a trade-off between accuracy and robustness in high-order CFD solvers.
Recently, a feed-forward neural network to detect troubled-cells [3] showed its potential as a universal troubled-cell indicator without parameter tuning. However, it was also observed that it exhibits some erratic convergence rate for smooth flows, and its performance is not reliable enough to be extended onto realistic configurations with unstructured-mixed grids. To address this issue, we develop an accurate and robust troubled-cell indicator using decision tree classifiers that can handle unstructured-mixed grids. Training data are generated by projecting the smooth and discontinuous analytic functions onto DG polynomial space. In the modal DG framework, we introduce input features that handle unstructured-mixed grid systems by exploiting the information of high-order shock-capturing schemes. Our tree-based models perform the binary classification, i.e. smooth or shock regions, using high-order features defined on compact stencil. Combined with proven limiting algorithms, we validate our tree-based models in terms of accuracy, robustness, and cost-efficiency on various grid systems. Though extensive numerical tests including shock-vortex interaction, we confirm that the proposed data-driven indicator not only provides the expected order-of-accuracy for vortex region but also flags the troubled-cells accurately and robustly for flow problems with shock-vortex structures.

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Advances in numerical methods for solution of PDEs
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CHARACTERIZATION USING BEAM-SOIL RESPONSES: A FULL-WAVEFORM INVERSION APPROACH

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ABSTRACT

This study presents a full-waveform inversion (FWI) method that utilizes measured deflections to reconstruct the material profiles of a beam-soil system, such as water pipelines supported by the soil. The forward problem for calculating the beam's deflection in the time domain can be formulated by the Euler-Bernoulli beam and the Winkler foundation models. The accuracy of the forward responses was validated by comparing them with ANSYS solutions. The dispersion characteristics of the flexural waves in the beam-soil system were also demonstrated considering various soil stiffness conditions. The inverse problem for reconstructing the material profiles of the beam-soil system can be formulated by a PDE-constrained optimization approach. The target inversion variables are the beam's elastic modulus and the soil's stiffness of the Winkler foundation model. The optimization approach seeks to minimize an objective functional comprising the least-squares misfit between measured and calculated deflections and regularization terms. By enforcing the stationarity conditions of a Lagrangian, Karush-Kuhn-Tucker conditions consisting of state, adjoint, and time-independent control problems are derived. The three problems are iteratively solved in the reduced space of control variables to reconstruct the beam's elastic modulus and the soil's stiffness. In numerical examples, three cases are presented: (1) inversion for the beam's elastic modulus while knowing the soil's stiffness, (2) inversion for the soil's stiffness while knowing the beam's elastic modulus, (3) simultaneous inversion for both the beam's elastic modulus and the soil's stiffness. In particular, it is shown that the two profiles can be simultaneously reconstructed using a single set of measured beam-soil responses. The methodology presented in this study can be used for various engineering applications, such as damage assessment of lifeline structures.

Model order reduction for parametrized continuum mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICS-BASED MANIFOLD REPRESENTATION USING DIFFUSION MODEL FOR COMPUTATIONAL MULTISCALE STRUCTURAL PROBLEMS

Hyejin Kim[*1], Seongwoo Cheon[1] and Haeseong Cho[1]*

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ABSTRACT

Computational multiscale homogenization method has proven to be a favorable strategy for characterizing an effective continuum model for heterogeneous composites at the microscopic level. This approach can also be extended to a multilevel finite element method known as the FE2 method. However, the presence of nonlinear behavior in heterogeneous composites introduces significant computational costs and necessitates recursive computation, given the intricate deformation mechanisms that connect different scales. Considering these challenges, implementing a reduced-order model to address the associated computational inefficiencies can be applicable. In this study, we propose a surrogate model designed to efficiently predict both global and local nonlinear behaviors within the microstructure, leveraging a reduced-order model based on a deep learning network model. Additionally, we explore the manifold representation of microstructure exhibiting nonlinear behavior by introducing a diffusion model, which bridges the inherent homogenized macroscale physics data governing microstructure evolution. Specifically, an autoencoder (AE) is applied as part of the deep learning-based reduced order model, effectively dealing with the high-dimensional quantities of interest in microstructure analysis and learning manifold representation. Furthermore, a flow-based diffusion model is employed to describe the relationship between the manifold representation of microstructure and the underlying physics of homogenized macroscale data.

Fracture, damage and failure mechanics of cementitious materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

QUANTIFICATION OF CONTRIBUTIONS ON PLASTIC SHRINKAGE CRACK WITH EVALUATION OF BLEEDING AND EVAPORATION

Hyun-Kyoung Kim[*1] and Hyo-Gyoung Kwak*[1]

[1]*KAIST*

ABSTRACT

Plastic shrinkage crack is a early plastic crack of concrete that occurs due to rapid moisture loss from fresh concrete and the tensile shrinkage following after that. Plastic shrinkage crack have a unfavorable influence on not only exterior appearance but also concrete structure in long term by corroding interior of concrete. Despite of the importance of preventing Plastic shrinkage crack in terms of maintenance, the numerical research and precautions on plastic shrinkage crack and its control is insufficient. This study is devoted to numerical analysis of bleeding and evaporation which are two measures of plastic shrinkage crack, and proposed quantification of the effect of each influencing factors including representative concrete curing method for plastic shrinkage crack, windscreen. For this purpose, bleeding was modelled by large consolidation theory, and the bleeding properties of concrete was determined by the regression on concrete mix variables to the normalized bleeding coefficients, together with the bleeding coefficient of reference concrete mix. And to evaluate evaporation, evaporation rate diminishing effect and concentration weighed characteristic velocity by CFD-analyzed wind profile was adopted to get better evaporation estimation than existing ACI nomograph. In the end, the proposed ready-made quantification of each influencing factor on surface dry time is expected to be effectively utilized in keeping plastic shrinkage crack in construction site.

Multiscale computational and data-driven approach of advanced materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MULTISCALE BRIDGING APPROACH TO PREDICT FRACTURE TOUGHNESS AND CRACK PROPAGATION CHARACTERISTICS OF POLYMER NANOCOMPOSITES

Jae Hun Kim[*1], Haolin Wang[1], Jihun Lee[1] and Hyunseong Shin[1]*

[1]*Inha university*

ABSTRACT

In this study, we proposed a multiscale bridging approach combined with molecular dynamics (MD) and finite element homogenization (FEH) method to predict fracture toughness and crack propagation characteristics of polymer nanocomposites. It has been reported that the precise characterization of the interphase elasto-plastic constitutive law is critical for predicting fracture toughness, fatigue crack growth, and overall strength of polymer nanocomposites [1, 2]. To characterize the interphase elasto-plastic properties, we employed full atomic molecular dynamics simulations and finite element homogenization analysis with a three-phase equivalent model that reflects the interphase between the nanoparticle and the polymer matrix. The interphase elasto-plastic properties were used to predict the fracture toughness of polymer nanocomposites by considering debonding between the particle and the interphase, as well as void growth. Additionally, we compared mode I and mode II crack propagation characteristics using phase-field finite element method.

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Imaging and computational methods for biomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PATIENT-SPECIFIC IN VIVO ESTIMATION OF BASILAR ARTERIAL LOCAL WALL DEFORMATION AND STIFFNESS USING A NOVEL IMAGING-IGA COMPUTATIONAL APPROACH

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ABSTRACT

A comprehensive understanding of the biomechanical behaviors and failure mechanisms of the basilar artery (BA) and its aneurysms is crucial for advancing disease diagnosis and treatment. In the current study we developed an image-based approach for the in vivo direct determination of basilar arterial wall deformation and stiffness. We start by using a novel MRI based imaging technique to extract the BA endoluminal geometry in humans over the cardiac cycle. Using the resulting segmented point-cloud data we reconstructed the three-dimensional endoluminal surface using non-uniform rational B-splines (NURBS). Using the local support mathematical feature of NURBS, we then estimated the BA endoluminal surface strain throughout the cardiac cycle. To determine the corresponding wall stresses, we developed a computational mechanics framework that incorporates membrane shell theory to estimate BA wall tension through the cardiac cycle. This method ignores bending and transverse shear deformation due to the thin wall of the artery. The membrane shell theory exploits static determinacy, allowing wall tension determination solely from considerations of geometry and blood pressure. A significant advantage of this approach is the elimination of the need for a material model or prior knowledge of residual stress and referential state of the BA wall. To numerically solve membrane shell equations and address complex geometry with higher-order continuity, we employ Isogeometric Analysis (IGA). In this process, the NURBS surface serves as input for the analysis, and IGA determines wall tensions from the geometry. We have developed a robust and open-source finite element framework utilizing FEniCS. The integration between FEniCS and NURBS is seamlessly facilitated through tIGAr, which is a Python library to perform IGA within FEniCS environment. Results from three human patients show several interesting features, such as regional large deformations that occurred in a peristaltic fashion, mechanical behaviors in the functional range demonstrated clear anisotropy and anatomical location differences. This imaging-IGA computational approach holds promise for improved insights into the dynamic behavior of intracranial arteries, contributing to enhanced diagnostic capabilities in neurovascular assessments.

ACCELERATED AND STABLE KRIGING SURROGATE MODEL TECHNIQUE FOR TRAINING LARGE-SCALE DATA

Jieon Kim[*1] and Gunwoo Noh[1]*

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ABSTRACT

Surrogate models, rapidly predicting response values based on design variable conditions, are essential for effectively executing engineering design, improvement, and optimization processes. Among these, the Kriging model is widely utilized because it offers both high prediction accuracy and provides statistical prediction uncertainty information at arbitrary locations. When training the Kriging model, it is necessary to solve the global optimization problem of the likelihood function based on the correlation matrix. Hence, when dealing with large-scale data, increasing the size of the correlation matrix leads to higher training costs and a greater unstable training outcome. This is a primary reason why, despite the high accuracy and utility of Kriging, it is not effectively utilized for large-scale data. In this study, we have developed a new approach called ASTEK (Accelerated and Stable Technique for Efficient Kriging) to overcome these challenges, ensuring consistently high accuracy and training efficiency regardless of data scale.

ASTEK consists of two stages: the ‘Preparation: offline’ and ‘Training’. In the ‘Preparation: offline’ stage, it pre-trains the ‘Optimal hyperparameter predictor’ with Artificial Neural Network and additional two more methods, Radial Basis Function Networks and Kriging, based on the data distribution and trends of the prepared sample pool. We applied the Ensemble of surrogates approach to select the most appropriate model for the given data, ensuring the accuracy and robustness of the 'Optimal hyperparameter predictor’.

In the ‘Training’ stage, where, upon input of arbitrary training data, it quantifies the distribution and trends as the same parameters in ‘Preparation: offline’ stage. These parameters are then applied to the ‘Optimal hyperparameter predictor’ and generate the Kriging model instantly.

In this study, we validate the effectiveness of ASTEK in significantly reducing training time while ensuring stable high accuracy for large-scale data through various numerical test problems and engineering examples. This is expected to contribute to effectively training and optimization works for large-scale data, addressing the challenges in ensuring accuracy and training efficiency that were previously encountered with traditional surrogate models.

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Modeling and simulation of advanced manufacturing processes for metals
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

OPTIMIZATION OF IRON POWDER COMPACTION PROCESSES USING DISCRETE ELEMENT AND MULTI-PARTICLE FINITE ELEMENT METHODS COUPLED WITH ARTIFICIAL NEURAL NETWORKS AND GENETIC ALGORITHM

Ji Hoon Kim[*1], Hossein Ghorbani-Menghari[1] and Majid Mohammadhosseinzadeh[1]*

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ABSTRACT

The compaction of powder plays a crucial role in diverse industries, including pharmaceuticals, ceramics, and metallurgy, where it transforms loose powder into a solid compact through mechanical forces. The integrity and quality of the compact are affected by several factors, such as the particle size distribution, compaction pressure, and powder flow properties. This study focuses on optimizing the quality of iron powder compacts. To achieve this, the discrete element method (DEM) and the multi-particle finite element method (MPFEM) were employed. In developing the numerical procedure, the impacts of the finite element size, the dimensions of representative volume elements, frictional forces, and springback were analyzed. The effectiveness of this combined DEM-MPFEM approach was verified for various powder size distributions. Subsequently, the data generated from this procedure was utilized to train an artificial neural network model. A genetic algorithm-based optimization was then applied to identify the most suitable powder size distribution for optimal quality of the compacted iron powder.

Emerging topology and shape optimization techniques in computational design of materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TWO-SCALE SHAPE AND TOPOLOGY OPTIMIZATION USING LEVEL-SET AND HEURISTIC METHOD WITH STRESS AND VOLUME CONSTRAINTS

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ABSTRACT

This paper presents a two-scale shape and topology optimization method using the level-set method and heuristic update scheme under stress and volume constraints. The optimization problem can be expressed as the Lagrange functional consisted with a compliance, linear elastic equilibrium equation and stress and volume constraints with Lagrange multipliers. The p-norm stress is introduced to analyze the sensitivity to stress constraint and the macro scale sensitivity can be obtained by solving adjoint equation. Two level-set function are introduced to define macro and micro structure. The macro structure is created based on the initial macro level-set function and updated by solving the reaction-diffusion equation. The micro structure is defined by a basic level-set function which determine the topology of the micro structure and the height of the macro element which change the shape of micro structure. Each finite element of the macro structure is considered as one micro structure. For each macro element, the energy-based homogenization method is applied to obtain the homogenized elastic tensor. The heights are updated by heuristic updating scheme with the parameter obtained from the optimal condition.

Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MECHANICAL BEHAVIOR ANALYSIS OF ADDITIVE MANUFACTURED CEMENTITIOUS MATERIAL BASED ON MICROSTRUCTURAL CHARACTERISTICS

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ABSTRACT

In the construction and building industry, additive manufacturing (AM) or 3D printing of concrete is widely studied. The AM process offers the advantage of rapidly printing irregular structures. Compared to conventional construction methods, AM structures exhibit interfaces between printed layers and filaments, inducing anisotropy. It significantly impacts directional mechanical properties [1]. Consequently, it is necessary to consider the interfacial effects on the responses when evaluating the AM structure behaviors.

This study examines the influence of the additive manufacturing process on the mechanical properties of cementitious materials, focusing on their microstructural characteristics. Micro-CT images facilitate effective investigation of phase distribution without material defects. The spatial distribution characteristics of the printed structure were examined in a probabilistic manner. A 3D microstructure (or virtual model) with the actual features was generated based on the CT images. The model was utilized to examine mechanical properties through simulation.
For the simulation, two types of the virtual models were designed to analyze the interfacial effects on the mechanical properties of the additive manufactured cementitious material: one is inter-layer model, and the other is inter-filament model. Using the crack phase field fracture model based on the finite element method [2], the responses, i.e., stiffness and strength, of each model were examined. The results indicated a strong correlation between the properties of the printed structure and pore distribution characteristics. Directional behaviors were investigated and correlated with microstructural characteristics.

It was found that the inter-layer less significantly affects the tensile behavior of the printed structure. Cracks under loading mainly propagated through inter-filament pores, which is continuously connected along printing direction. By combining microstructural characteristics and mechanical properties via virtual experiments, an optimized printing pattern can be suggested to improve the integrity of the printed structure.

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Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT OF A FATIGUE DAMAGE ASSESSMENT METHOD BASED ON THE SMALL PUNCH TEST

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ABSTRACT

In recent years, energy scarcity and greenhouse gas reduction have become important global issues. Thermal and nuclear power plants are responsible for a significant portion of energy generation. From a thermodynamic perspective, a 10 degrees Celsius increase in steam temperature results in a 0.5% increase in power generation efficiency. In addition, a 9% increase in power generation efficiency results in a 20% reduction in greenhouse gas. Next-generation power plants aim to increase power generation efficiency and reduce greenhouse gas emissions by increasing steam temperature. However, it is crucial to understand the mechanical properties of structural materials, such as tensile, creep, and fatigue, to safely operate plants with higher steam temperatures for extended periods of time.

Mechanical properties, such as tensile, creep, and fatigue, are typically evaluated through uniaxial test (UT). This method directly stresses the specimen to measure its mechanical properties. The strain value at a given stress is directly derived since the deformation of the specimen occurs under uniaxial stress. Therefore, UT is a useful method for characterizing the mechanical properties of materials. However, it has a fundamental limitation in that it is resource-intensive and time-consuming to obtain test results.

To address the limitations of UT, small punch test (SPT) has been proposed as an alternative. SPT has the advantage of using a very small specimen size, which consumes very little material and requires relatively little time to obtain test results. Unlike UT, which measures strain and stress, SPT measures displacement and load. Thus, to evaluate the mechanical properties of materials using SPT, it is crucial to establish a correlation between the two test methods.

Unlike UT, which applies direct stress to the specimen, SPT applies indirect stress through the punch and punch ball. Additionally, while UT deforms the specimen under uniaxial stress state, SPT deforms the specimen under multiaxial stress state. This difference in loading mechanism makes it challenging to establish a correlation between the two test methods. Although several researchers have established the tensile and creep properties of SPT, its fatigue properties have not been clearly established.

Thus, the objective of this study is to create a method for assessing fatigue damage using SPT. A model for analyzing fully reversed fatigue damage is developed based on finite element analysis (FEA), and S-N curves are derived using only SPT. The study's validity was confirmed by comparing the simulation results with the S-N curves obtained from the actual UT.

Modeling, simulation, and AI for ultrasonic NDT and SHM
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ANALYSIS OF CROSS-SECTIONAL LOAD ACCORDING TO ASYMMETRIC FORMATION OF 3-D RC RAHMEN STRUCTURE

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ABSTRACT

When performing numerical analysis of a 3D structure, the analysis is generally conducted based on symmetrical shapes. However, currently, various structures have asymmetrical shapes. When designing these asymmetric structures, the main structure part of the lower part of the structure and the substructure part of the upper part have different behavior than when numerically analyzing symmetrical structures. Accordingly, the distribution ratio and value of the load received by each structural part also change. This study will analyze the change in load received by structural members when a symmetrical structure changes to an asymmetrical structure. Based on the 20-story structure, analysis of symmetrical and asymmetrical structures will be conducted, and in asymmetrical structures, changes according to the shape and location of the substructure and the ratio of the main structure and substructure will be considered. In this process, numerical analysis will be performed considering the construction sequence of the structures to maximize the behavior of the actual structure. By analyzing asymmetric structures in 3-D considering the construction sequence, we will enable efficient selection of cross-sectional settings of members during construction of the structure.

Multiscale computational and data-driven approach of advanced materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN MULTISCALE FINITE ELEMENT METHOD USING DEEP NEURAL NETWORK COMBINED WITH PROPER ORTHOGONAL DECOMPOSITION

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ABSTRACT

A data-driven multiscale finite element method (FE2) utilizing deep neural network (DNN) and proper orthogonal decomposition (POD) has been proposed to characterize the behavior of composite materials, including nonlinear and heterogeneous materials. The data-driven FE2 approach assigns data to all integration points to satisfy microscopic equilibrium and resolves the macroscopic problem. We enhance the efficiency of database construction by pre-computing the microscopic problem of the representative volume element (RVE) and incorporating POD to develop a precise and efficient DNN model for predicting microscopic behavior. Therefore, we have further improved the data-driven FE2 technique by efficiently generating an available database. In the numerical example, we effectively attained accurate results for both macroscopic and microscopic analyses with sparse dataset. Employing a data-driven FE2 based on the DNN-POD approach, the methodology not only exhibited its ability to overcome data scarcity but also demonstrated a high degree of accuracy in predicting outcomes at both scales. This work is believed to have significantly increased the efficiency of computational structural mechanics.

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Recent developments in peridynamics modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PERFORMANCE INVESTIGATION OF DIFFERENTIAL OPERATORS IN THE PERIDYNAMICS FORMULATION FOR HEAT CONDUCTION ANALYSIS

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ABSTRACT

Differential operators in the formulation of the peridynamics are obtained from the peridynamic functions, and the precision of the spatial derivatives is contingent on the appropriate selection of the peridynamic function. We investigate the performance of the thermal peridynamic formulation by changing the order of peridynamic functions in the form of Taylor series expansions and weight functions. Six different orders of the Taylor series expansions as well as three individual weight functions are tested to evaluate the performance of the peridynamic functions. For each function, m-convergence test is performed by decreasing the peridynamic point spacing while keeping a specific horizon size. For a one-dimensional case, the heat distribution and fluxes are calculated by integrating the peridynamic functions in quasi-static and transient analyses. Subsequently, the function demonstrating the best performance in this one-dimensional case is employed to solve the three-dimensional quasi-static heat conduction problem. The weight function influences the heat flux calculation across all orders, and the effect considerably decreases at the second order, yielding accurate heat fluxes. Furthermore, in the second-order formulation, the chosen weight function enhances the accuracy of heat flux calculations. Utilizing this optimized combination of second-order formulation and weight function, the temperature and heat flux fields in three dimensions are in good agreement with those calculated in the finite element analysis. This peridynamic formulation proves versatile for various thermodynamic problems, offering high accuracy in heat conduction analyses.

Recent advances in high-order methods for computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADAPTIVE SUBCELL SHOCK-CAPTURING FOR DISCONTINUOUS GALERKIN METHODS ON SUPERSONIC AND HYPERSONIC FLOWS

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ABSTRACT

A novel subcell shock-capturing approach is proposed to enhance the performance of discontinuous Galerkin (DG) method on supersonic and hypersonic flow simulations accompanying strong physical discontinuities. High-order methods (HOM), receiving much attention in scale-resolving simulations due to low numerical dissipation and high scalability, have the potential to predict heat transfer rate more accurately than the second-order finite volume method (FVM) in hypersonic simulations. This requires an accurate and robust shock-capturing as an essential pre-requisite because HOM are in general much more susceptible to numerical Gibbs oscillations in the vicinity of strong shock waves. While the posteriori subcell limiter [1] demonstrated the robustness favorable to hypersonic flow simulations, it suffers from Gibbs oscillations as well when subcell FVM solutions are directly used to reconstruct a high-order solution, leading to the loss of accuracy especially in steady-state simulations. In order to address this issue, we design a novel oscillation-detecting process to identify Gibbs oscillations in the reconstruction step by analyzing subcell FVM solutions and reconstructed high-order solutions. We then retain the subcell FVM solutions without further proceeding high-order reconstruction if oscillations are detected during the reconstruction step. The subcell FVM solutions are updated via the boundary fluxes reconstructed using the DRM-DG method [2, 3]. This hybrid approach enables the high-order flux-interaction between the subcell FVM solutions and the neighboring DRM-DG solutions. From extensive numerical experiments, it is verified that the proposed method effectively eliminates numerical oscillations during the reconstruction and accurately resolves shock waves on supersonic and hypersonic flow simulations.

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Advanced materials: Computational analysis of properties and performance
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FRACTURE STUDY OF SINGLE CRYSTAL SILICON USING ATOMISTIC SIMULATIONS

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ABSTRACT

Silicon is the most commonly used semiconductor material and has played a key role in the recent advances in nanotechnology as a building material for MEMS (micro-electro-mechanical systems). As the size of silicon-based devices continues to decrease to sub-micrometer levels, it becomes of critical importance to have a thorough understanding of fundamental deformation mechanisms since materials on small length scales often exhibit completely different behaviors from their bulk counterparts. For example, while silicon is an inherently brittle material, several recent experiments have shown that micrometer-scale devices made of single crystal silicon exhibit plastic deformation at room temperatures. In the present work, the fracture behavior of single crystal silicon is investigated using atomistic simulation methods. Atomistic simulation is one of the most suitable tools to understand the exact nature of silicon, but the outcomes are strongly tied to particular interatomic potentials used in the simulation. In this study, we considered three interatomic potential models for silicon: (1) Stillinger-Weber (SW), (2) Modified Embedded Atom Model (MEAM), and (3) ReaxFF. The simulation mimics the mode-I fracture test for those models in five different crystallographic orientations and with various initial crack sizes as well as the different model sizes. The simulation results show two different failure modes of the crystal: (1) a slip deformation along the (111) plane or (2) a crack propagation in the perpendicular direction to the loading. It is found that the various input parameters as well as the interatomic potential models affect these failure behaviors with the SW silicon model the most ductile among the tested potential models although the SW model also shows the brittle fracture in certain orientations. The mechanisms leading to the different failure behaviors are identified and some material parameters are computed for each potential model to predict the failure behavior.

Multiscale computational and data-driven approach of advanced materials and structures
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COMPUTATIONAL INTERPRETATION OF SHAPE MEMORY EPOXY: PROCESSING AND ITS OPERATION

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ABSTRACT

The shape forming and restoration mechanisms of shape memory epoxy originate from the molecular-scale dynamics that epoxy molecules undergo during thermomechanical processes. In this study, the microstructural changes that occur at the molecular scale caused by heat and load during the programming and operation of the epoxy network were investigated using molecular dynamics simulations. The mechanical behaviors of each molecule were analyzed by classifying it into translation, rotation, and deformation based on the classical kinematic framework. Specifically, depending on its structural properties, each molecular component was rearranged to different levels, forming local residual stresses. The principle leading to shape recovery as the subsequent thermal load breaks the equilibrium of residual stresses and resulting changes in the mechanical anisotropy of entire epoxy network were also analyzed through a subcontinuum perspective. This study has the potential to be extended to a method for designing epoxy resins that satisfy desired physical properties and shape recovery performance.

Computational mechanics for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EMPLOYING THE GURSON-TVERGAARD-NEEDLEMAN MODEL TO PREDICT DUCTILE FRACTURE IN METAL ADDITIVE MANUFACTURING

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ABSTRACT

Metal Additive Manufacturing (Metal AM), commonly known as 3D printing, is a rapidly evolving industry with significant implications across various sectors. This technology is acclaimed for its customization capabilities, cost-efficiency, and environmentally friendly production processes. In particular, Metal AM is revolutionizing the way metallic components are fabricated. However, a notable challenge associated with Metal AM is the potential reduction in durability and strength of parts compared to those produced by traditional manufacturing methods. This weakness is often attributed to defects such as porosity and inclusions in the Heat Affected Zone (HAZ) during the printing process. This study addresses the critical issue of ductile fracture in Metal AM parts by employing the Gurson-Tvergaard-Needleman (GTN) model, a widely utilized numerical method for modeling ductile fracture phenomena. The GTN model is particularly effective in simulating the initiation, growth, and coalescence of microvoids and cavities in metallic materials, leading to fracture. By adapting the GTN model to the specific context of Metal AM, this paper presents a comprehensive approach to understanding and predicting the ductile fracture behavior of Metal AM materials. Our research involved extensive computational simulations and experimental validations, focusing on the microstructural characteristics unique to Metal AM. The findings offer valuable insights into the fracture mechanisms of Metal AM parts and provide a robust framework for predicting their structural integrity. This model not only enhances the understanding of the mechanical properties of Metal AM materials but also serves as a critical tool for optimizing the AM process, thereby contributing to the advancement of this transformative manufacturing technology.

AUTOENCODER-BASED GAPPY DATA RECONSTRUCTION ALGORITHM

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ABSTRACT

In this study, we have developed a data reconstruction algorithm called Gappy Autoencoder (Gappy AE) to overcome the limitations of digital twins caused by sparse measurements or missing data in the digital twin model. The existing methodology for data reconstruction using Proper Orthogonal Decomposition (POD), known as Gappy POD, is being utilized. However, the Gappy POD approach has limitations in representing solutions with large Kolmogorov N-width due to its ability to predict data only within the linear subspace. On the other hand, utilizing unsupervised learning models based on nonlinear manifolds provides superior data representation capabilities compared to the linear subspace. An autoencoder model is trained and the decoder part constructs the nonlinear manifold that maps low dimensional latent vectors to high dimensional input data. In this research, we propose a more generalized methodology called Gappy AE, which utilizes nonlinear manifolds (i.e., decoder parts of trained autoencoders) to represent data that the conventional Gappy POD approach cannot handle effectively. This can be applied in real-time state prediction based on measured values. Through numerical examples of 2D diffusion and 2D wave equation problems, we have confirmed that Gappy AE outperforms Gappy POD in terms of data reconstruction performance when sparse measurements on boundaries are given. Furthermore, we evaluate how data reconstruction accuracy is influenced by three different sampling algorithms: discrete empirical interpolation method, the S-OPT algorithm, and uniformly distributed sampling.

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Advanced discretization schemes and solution strategies for computational structural dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MULTI-DIRECTOR CONTINUUM BEAM FINITE ELEMENT FOR WIRE ROPE STRANDS

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ABSTRACT

This study introduces a finite element model for the analysis of wire rope cables, specifically designed to efficiently handle their complex geometry. The model is based on continuum mechanics principles and employs multi-directors and cross-sectional elements to accurately represent the double helical structures of the individual wires within the wire rope strands. The main advantage of this continuum beam formulation is its ability to address intricate wire rope geometries and inter-wire movements within a simplified beam framework, regardless of the number of strands and constituent double helical wires. This approach offers both ease of modeling and efficient analysis while accounting for geometric complexities. Additionally, the proposed beam element model exhibits high accuracy while requiring significantly fewer degrees of freedom compared to traditional three-dimensional solid finite element models commonly used for cable analysis. To validate the effectiveness of our proposed model, we conducted several numerical examples. These examples show the robustness of the model in accurately simulating the physical behaviors of wire rope cables under various conditions. They also demonstrate the efficiency and reliability of the model in analyzing the complexities of wire rope cable systems.

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ADAPTIVE MESH REFINEMENT STRATEGIES FOR MELT POOL RESOLUTION IN PART-SCALE AM SIMULATIONS

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ABSTRACT

The computational expense of part-scale laser powder bed fusion (LPBF) simulations can be drastically reduced by leveraging data contained in the prescribed beam scan path. This information provides times and locations where large thermal gradients, melt pools, and other small-scale phenomena are likely to develop as the beam traverses the work piece. The mesh in these regions can be selectively refined and coarsened as the beam passes over, allowing fine resolution of the melt pool dynamics while minimizing the number of cells and resources required for the problem. An adaptive mesh refinement (AMR) technique was developed to exploit this information within the open-source LBPF modeling tool, AdditiveFOAM. The implementation makes full use of existing AMR and load balancing capabilities available in OpenFOAM, upon which AdditiveFOAM is based. The proposed approach uses scan path information to generate a marker field which is provided to the mesh refinement library. This marker field is created by dividing the simulation into a specified number of intervals. At the beginning of each interval, the algorithm marches forward along the scan path and searches for any cells which overlap with the beam spatial dimensions, until the end of the interval is reached. Overlapping cells are marked for refinement, so that the beam behavior is captured on a fully refined grid as it progresses through the interval.

The performance of this approach is examined for small- and part-scale simulations on both HPC and edge computing resources. Time profiling studies demonstrate that for a given case, there exists an optimum number of refinement intervals which balances frequent AMR operations against long linear algebra solves resulting from over-refinement. A preliminary scaling study indicates that the proposed strategy achieves acceptable results on HPC resources; however, the true impact of this approach is to significantly reduce the resources required for a problem. As an example, one non-AMR benchmark case with a fine mesh required 27 minutes to complete on several HPC nodes. The same problem was finished in 8 minutes using an ordinary laptop with the proposed AMR strategy, with minimal difference in results.

Modern structure-preserving methods for PDEs
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HIGH-ORDER BOUNDS-SATISFYING APPROXIMATION OF PARTIAL DIFFERENTIAL EQUATIONS VIA FINITE ELEMENT VARIATIONAL INEQUALITIES

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ABSTRACT

Solutions to many important partial differential equations satisfy bounds constraints, but approximations computed by finite element or finite difference methods typically fail to respect the same conditions. Chang and Nakshatrala enforce such bounds in finite element methods through the solution of variational inequalities rather than linear variational problems. Here, we provide a theoretical justification for this method, including higher-order discretizations. We prove an abstract best approximation result for the linear variational inequality and estimates showing that bounds-constrained polynomials provide comparable approximation power to standard spaces. For any unconstrained approximation to a function, there exists a constrained approximation which is comparable in the $W^{1,p}$ norm. In practice, one cannot efficiently represent and manipulate the entire family of bounds-constrained polynomials, but applying bounds constraints to the coefficients of a polynomial in the Bernstein basis guarantees those constraints on the polynomial. Although our theoretical results do not guaruntee high accuracy for this subset of bounds-constrained polynomials, numerical results indicate optimal orders of accuracy for smooth solutions and sharp resolution of features in convection-diffusion problems, all subject to bounds constraints.

Advances in material model calibration for computational solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

UNVEILING FULL-FIELD MODULUS AND STRESS USING DIGITAL IMAGE CORRELATION

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ABSTRACT

Digital Image Correlation (DIC) is a widely used technique in experimental labs for assessing full-field displacement. However, its potential extends beyond this setting. This presentation advances the possibilities of characterizing a spatially varying modulus field by integrating DIC with a partial differential equation (PDE)-based inverse problem, forming a unified joint inversion. With images and boundary conditions it will be shown that displacement and modulus fields can be discovered, naturally extending to stress fields. The PDE describes the expected forward physics; this presentation will show examples with linear elasticity and hyperelasticity. Our exploration reveals that handling the joint inverse problem within an infinite-dimensional framework (using adjoint-based gradients and Hessians) allows for the emergence of heterogeneity or defects in the solution. We will present results from various regularization methods, incorporated to mitigate the ill-posed nature of the inverse problem. Notably, total variation (TV) will be highlighted for its effectiveness in preserving sharp interfaces found in various materials like fibers, particles, and grain boundaries. The presentation will elaborate on a primal-dual TV formulation designed to maintain mesh-independence. Finally, we will discuss inversion results obtained from experimental coupons 3D printed via Polyjet, where the as-printed color corresponds to modulus. To the best of our knowledge, the algorithm presented here represents a pioneering effort in inferring modulus as a fully heterogeneous parameter.

Recent advances in discretization techniques for coupled problems in incompressible fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A PRESSURE-ROBUST HYBRIDIZED DISCONTINUOUS GALERKIN METHOD FOR THE CAHN-HILLIARD-NAVIER-STOKES SYSTEM

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ABSTRACT

Diffuse interface models are an increasingly popular approach to the simulation of multiphase flow phenomena. From the computational point of view, the advantage of these models is the elimination of the need to track the interfacial dynamics between phases. This advantage, however, comes at the expense of the solution of an additional nonlinear parabolic equation arising from thermodynamic considerations. One such example is the fourth-order Cahn-Hilliard equation describing the phase separation of an immiscible binary mixture, which, when coupled to the incompressible Navier-Stokes equations, can serve as a model for immiscible two-phase flow in porous media at the pore scale.

An effective approach to the numerical solution of the Cahn-Hilliard equation involves transforming it into a coupled system of second order equations and applying an interior penalty discontinuous Galerkin (DG) method. Among many other advantages, the DG method enjoys local mass conservation due to the introduction of numerical fluxes across element interfaces; however, the tradeoff is an increase in computational expense in comparison to conforming finite element methods. On the other hand, much of the recent progress in the numerical solution of incompressible flow problems has concentrated on pressure-robust finite element methods, a class of methods that preserve a fundamental invariance property of the incompressible Navier-Stokes equations. Two essential ingredients are required for pressure-robustness: exact enforcement of the incompressibility constraint, and H(div)-conformity of the finite element solution.

For this reason, we propose and analyze a hybridized interior penalty discontinuous Galerkin (HDG) method to solve the Cahn-Hilliard-Navier-Stokes system wherein additional finite element spaces are introduced on the interfaces between mesh elements. By enforcing a suitable transmission condition on the numerical flux, the degrees of freedom on the interior of each element can be eliminated through static condensation. This reduces the size of the globally coupled algebraic system compared to the standard interior penalty method while preserving its many advantages. Moreover, H(div)-conformity of the discrete velocity solution is enforced through the introduction of a pressure facet variable, ensuring the numerical scheme is pressure-robust. To guarantee unconditional stability of the numerical scheme and unique solvability of the resulting nonlinear algebraic system, we employ a standard convex-concave splitting of the nonlinear chemical energy density and a first order implicit Euler time integration scheme.

Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MIXED PARTITION OF UNITY METHODS AND STOCHASTIC GILLESPIE ALGORITHMS FOR TRANSPORT-REACTION EQUATIONS

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ABSTRACT

We propose to solve Transport-Reaction Problems in a new partially deterministic (continuum part) and partially stochastic framework (finite size part). We couple a PDE defined on a domain Ω and a Gillespie algorithm solving the discrete finite-size particle system reaction part of the problem.

The idea of discretisation is simple, but novel, and is in both its theoretical and practical aspects of great importance. We interpret the solution of the PDE as a continuum probability distribution L_x in the space part of the problem, i.e L_x determines where in space to find particles at time t. Let $N = N(t) \in \mathbb{N}$ be the number of particles in the system at time t. We assume there exists a distribution transfer function, choosing the position of each particle from the spatial probability function. We allow here memory, i.e. there is knowledge about the previous positions. Note that this setting solves a lot of long-standing theoretical problems, like the property of infinite speed of propagation of the classical diffusion equation. The separation between transport and reaction allows for a number of interesting combinations of numerical methods. The reason for using a finite particle size has several advantages, finite size effects can be effectively investigated. Nonlinear reaction mechanisms are very common in many applications, like chemical reaction systems, biochemistry, epidemiology, population dynamics, opinion formation, mathematical finance, etc. The particles can undergo type transformations as given by transformation rules called reactions. The reaction process then is implemented numerically by the so-called Gillespie algorithm. The discretisation of the full process is a follows. For the transport PDE we could use any common discretisation method, finite differences, finite volumes or finite elements. We then have to attach reaction volumes to this underlying spatial discretisation. In finite differences, the reaction volumes are identical with the discrete mesh points. In finite elements we can define the reaction volumes with the help of basis functions. Here we propose to use generalised finite element methods based on partition of unity methods, as this allows us to cover complex spatial geometries. The discretised transport equation allows the computation of the particle distribution function L_x. The fluxes between reaction volumes can therefore be computed, establishing transport rules. Then we use a Gillespie algorithm for the reaction part. We can be improve the latter by using a generalised Gillespie algorithm with a decision tree relating to the spatial structure of the problem.

Next-generation numerical methods for coupled multiphysics problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VARIATIONAL MODEL AND NUMERICAL ANALYSIS OF FLUID IN POROELASTIC MEDIUM

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ABSTRACT

In this talk I will discuss modeling fluid flow through a deformable porous medium. I will introduce a system derived using energetic variational approach, discuss its comparison to an existing approach based on Biot's consolidation model, and present numerical methods and simulations based on it.

Numerical modeling of granular and multiphase flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HIGH SPEED COMPUTING FOR MIXING OF BI-DISPERSE PARTICLES IN A ROTATING DRUM

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ABSTRACT

Powder mixing is ubiquitous in a wide variety of manufacturing sectors including chemical industries. In the mixing process, multiple components with different physical properties such as particle size are usually treated. In these conditions, powder segregation can occur due to the difference in particle properties. Degree of segregation of powder mixture has a significant impact on the quality of the final product obtained by processing the powders, and thus methods to predict the degree of segregation are required. Computer simulation using the Discrete Element Method (DEM) is a powerful tool for the analysis of powder mixing process. In a DEM, dynamics (position and velocity) of an individual particles are numerically solved. These calculations are performed at extremely small time-step (micro seconds order). Therefore, a large number of iterations are required to calculate the entire powder mixing process, and it is difficult to predict a practical mixing in an actual process.

Recently, we developed an original machine learning model, namely recurrent neural network with stochastically calculated random motion (RNNSR), which allows long time scale powder mixing simulation with low computational cost and high accuracy [1]. RNNSR learns individual particle dynamics from short-time DEM simulation results and predicts a powder mixing for a long time. However, the RNNSR was only verified for mono-dispersed particles and has not been applied to bi-disperse particle systems that exhibit segregation. In this study, we expanded the RNNSR to handle bi-disperse particles and evaluated its effectiveness in simulating segregation phenomena. Development of this model significantly contributes to the implementation of powder simulations at powder properties and time scales closer to actual processes.

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Mathematical modeling and simulation for social, environmental, and disaster prevention issues
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EVALUATION OF EFFECTIVENESS OF TRAFFIC JAM ABSORPTION DRIVING USING COMPUTER SIMULATION

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ABSTRACT

Congestion-absorbing driving is known as an effective driving method for resolving traffic jams. Congestion-absorbing driving is based on the idea of reducing congestion by reducing excessive acceleration and deceleration while driving at low speeds while keeping a relatively large distance between vehicles. In this study, traffic jam absorption driving is applied to traffic simulation and its effectiveness is verified. The simulation results show that the average arrival time of the vehicle has become shorter. This shows that it is possible to increase the average speed in a congested area by not propagating deceleration to vehicles behind by driving to absorb congestion.

Mathematical modeling and simulation for social, environmental, and disaster prevention issues
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BAYESIAN TEMPORAL CONVOLUTIONAL NETWORK FOR EXCHANGE RATE PREDICTION

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ABSTRACT

This study proposes Bayesian Temporal Convolutional Network (BTCN) model applied to exchange rate prediction, and the performance of the proposed model is verified by conducting experiments on USD/JPY exchange rate data in 2018. The BTCN model applies the Bayesian neural network approach and Bayes by Backprop to the Temporal Convolutional Network(TCN) model, which improves the performance of the model for exchange rate forecasting compared to the TCN model by introducing an estimation for exchange rate uncertainty. The performance of the BTCN model on the exchange rate prediction task and the effect of the number of Monte Carlo approximation samples on the BTCN model are discussed separately in the experiments. For the exchange rate prediction experiments, the BTCN, TCN-with-dropout, and TCN-without-dropout models are trained separately. For comparing the prediction results of the three models, the BTCN model has a faster decrease in the value of the loss function on the validation dataset compared to the two TCN models, and the value of the loss function after the model is converged is smaller than the other models. The results of the experiments show that the BTCN model fits the true distribution better than the TCN model, and the introduction of uncertainty estimation has improved the ability of the model to search for optimal solutions.

SYMBOLIC REGRESSION AND EXTENDED PHYSICS-INFORMED NEURAL NETWORKS FOR GRAY-BOX MOTION EQUATION LEARNING

Elham Kiyani[*1], Khemraj Shukla[1], Mikko Karttunen[2] and George Karniadakis[1]*

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ABSTRACT

Partial Differential Equations (PDEs) are essential in dynamic system modeling across fields such as fluid dynamics, heat transfer, and phase transformations, aiding in understanding and predicting complex behaviors[1]. However, developing comprehensive models remains challenging. Our study introduces a novel framework using eXtended Physics-Informed Neural Networks (X-PINNs) [2] and symbolic regression [3] to reveal hidden components of nonlinear equations from data. X-PINNs, the foundation of our approach, employ a domain decomposition strategy in space- time, improving upon traditional methods by ensuring flux continuity across domain interfaces. The Allen-Cahn equation, pivotal in phase transition studies, validates our method's effectiveness.

Symbolic regression, integral to our framework, efficiently derives accurate mathematical formulas from data, identifying precise equations corresponding to specific datasets. It successfully predicts the explicit formulas of unknown equation terms.

To evaluate our framework's effectiveness in a setting that closely mimics the complexities of real-world data, we introduce random noise into our datasets and demonstrate the resilience of our framework when faced with substantial levels of noise, mirroring the often unpredictable and imperfect nature of real-life data conditions.

A critical finding is the minimal data needed for effective neural network training. We established that using at least 50% of the data is essential for correctly predicting dynamical equations, while a minimum of 60% is required for accurate unknown coefficient predictions.

Our approach, combining X-PINNs with symbolic regression, shows great promise in dynamic system modeling, effectively uncovering hidden equation aspects under challenging conditions of noise and limited data.

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Advances in computational biomechanics and mechanobiology
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE MODELING OF CALCIFIED POLYMER HYDROGELS

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ABSTRACT

Hydrogels, a significant group of highly hydrated polymers, represent the best choice for the potential application to bone fracture regeneration, which goes back to their bioactivity, affinity for biologically active proteins and compatibility with the bone tissue. However, this kind of materials also shows a serious disadvantage, namely, it loses its mechanical strength through swelling. This makes its straightforward usage difficult and motivates the development of different enhancement procedures. One of the most modern techniques for this purpose is calcification or, in a more general sense, mineralization. This method is inspired by the natural process of the bone growth where the enzyme alkaline phosphatase causes mineralization of the bone by cleavage of the phosphate from organic molecules. An analogous process induces homogeneous mineralization of a hydrogel and increases its mechanical strength. Recently, optical and electron microscopy has revealed that calcification yields different types of microstructure dependent on the type of the underlying polymer, and thus has clearly indicated that computational modeling can significantly contribute to the targeted investigation of effective behavior and material parameters. The current contribution uses the multiscale finite element method to simulate the effective material behavior of calcified hydrogels. Within this framework, representative volume elements (RVEs) are generated to depict the biphasic material microstructure consisting of the organic hydrogel and anorganic calcium phosphate [1]. Most commonly, the anorganic phase appears in the form of spherical inclusions or honeycomb grids where the characteristic size of a typical unit might vary. The approach proposed treats the calcified regions as linear elastic material and assumes the Ogden model for the hydrogel. Diffusivity is another important aspect in this context [2]. Its study requires a profound knowledge on the processes on the nanoscale. This time, the effective behavior is investigated by using the asymptotic homogenization approach.

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Advances and applications of polytopal methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STABILIZATION OF MIXED DISPLACEMENT-PRESSURE FINITE ELEMENTS AT FINITE STRAINS USING POLYHEDRAL FORMULATIONS AND VORONOI MESHING

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[1]RWTH Aachen University

ABSTRACT

The hexahedral mixed displacement-pressure finite element of the lowest order (H1/P0) has shown to be simple and effective during both linear and nonlinear analysis of incompressible solids. While the discrete displacement field is generally considered to be sufficiently accurate, the discrete pressure field can sometimes be heavily polluted by spurious pressure modes. This results from the fact that the element does not fulfill the inf-sup condition. While postprocessing techniques, such as pressure filtering or smoothing, exist to remove the spurious pressure modes from the solution, this contribution aims on the exclusion of spurious pressure modes from the solution a priori due to the element geometry. By employing polyhedral finite element formulations on Voronoi tessellations in three dimensions, we show that the discrete kernel of the linearized mixed bilinear form only consists of the hydrostatic pressure mode. A spurious pressure mode is automatically suppressed due to the vertex-to-volume ratio in the finite element mesh. These considerations hold for any arbitrary physically admissible displacement state that can occur within a Newton-Raphson framework. Both linear and nonlinear numerical examples show that spurious pressure modes are indeed suppressed if the type of tessellation is changed from hexahedral to Voronoi.

Data-driven methods for modeling complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STATISTICAL MECHANICS OF DYNAMICAL SYSTEM IDENTIFICATION

Andrei Klishin[*1], Joseph Bakarji[2], Nathan Kutz[1] and Krithika Manohar[1]*

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ABSTRACT

Recovering the dynamical equations from observed noisy trajectory data constitutes the problem of system identification. Approaches such as Sparse Identification of Nonlinear Dynamics (SINDy) are usually framed as minimizing a loss function that balances the data fit with parsimonious regularization, requiring a trial-and-error selection of hyperparameters. In this work we formulate system identification as a two-level Bayesian inference problem that explicitly separates variable selection from variable values and uses statistical mechanics techniques to compute the posterior parameter distribution in closed form and avoid Monte Carlo sampling. The low-data limit of this approach provides an uncertainty quantification of the identified models. The high-data limit resembles the thermodynamic limit and leads to a sharp sparsity- and noise-induced phase transitions between correct and incorrect identification. The statistical mechanics perspective can be integrated with other SINDy variants and applied to sparse regression problems in other contexts.

TOPOLOGY OPTIMIZATION OF THERMAL-ELASTIC STRUCTURES: CO-DESIGN OF GEOMETRY AND FUNCTIONALLY GRADED MATERIAL

Stefan Knapik[*1], Shiguang Deng[1], Liwei Wang[1], Jian Cao[1], Wing Kam Liu[1] and Wei Chen[1]*

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ABSTRACT

Recent developments in additive manufacturing have greatly enhanced our ability to fabricate functionally graded materials (FGMs), such as continuously graded alloys, providing unprecedented flexibility in structure design beyond discrete palettes of materials. FGMs hold tremendous potential for thermal-elastic applications, allowing for precise control over thermal and mechanical stress responses through tailored material properties. However, traditional topology optimization (TO) approaches cannot accommodate FGMs as they pre-assign material properties and segregate material selection as a distinct process. While multi-material TO approaches allow for voxel-level material composition design, they often fail to adequately consider crucial metallurgical factors like alloy compatibility. Similarly, existing thermal-elastic TO methods neglect or only partially consider the dependence of material properties on temperature.

We aim to address these gaps by developing more effective FGM design methodologies, integrating a density-based TO framework with automatic differentiation for improved computational efficiency and extensibility. This method enables the concurrent optimization of material distributions and geometric configurations. It utilizes a data-driven radial basis function interpolation to model material properties, facilitating continuously varying material combinations with minimal computational overhead. The inclusion of a penalization mechanism within the material interpolation scheme can deter the selection of unobserved material mixtures – a critical factor when accurate property interpolation is uncertain. A key feature of our method is the consideration of temperature-dependent material properties, a vital consideration for realistic design evaluation but largely overlooked in thermal-elastic TO approaches. This results in nonlinear thermal analyses for accurate temperature solutions, which are crucial since material properties can vary greatly with temperature. To ensure a robust design, we propose a unique stress constraint aggregation to efficiently manage spatially variable stress limits influenced by temperature and material composition.

A case study focusing on blisk design for aerospace applications demonstrates the multiple advantages of our approach. The continuous material design efficiently balances the interplay between temperature variation and mechanical stresses, achieving significant improvements over traditional discrete material design methods. It also successfully addresses the challenge of alloy compatibility by penalizing untested material combinations. Most notably, the holistic consideration of temperature-dependent material properties boosts the accuracy of our solutions, thereby enhancing design confidence. In addition to these benefits, our method contributes to sustainability by limiting the utilization of critical materials. These advancements collectively mark a significant stride in optimizing high-performance engineering structures while prioritizing performance, resilience, and environmental impacts.

Isogeometric methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ISOGEOMETRIC SHAPE SENSITIVITY ANALYSIS CONSIDERING TANGENTIAL DIVERGENCE OF NON-SMOOTH BOUNDARY IN BOUNDARY APPROACH

Keun-Hyeong Ko[*1], Hyun-Seok Kim[2] and Seonho Cho[1]*

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ABSTRACT

Despite the conventional finite element analysis (FEA) based boundary method for shape design sensitivity analysis (DSA) has the advantage of low computation costs, the accuracy of computed sensitivity is not satisfactory due to the inaccurate consideration of boundary geometry. To overcome this difficulty, employing an efficient adjoint method, we propose an isogeometric analysis (IGA) [1] based boundary method for shape DSA that can exactly handle the normal and curvature on a non-smooth boundary [2]. The accuracy can be improved by using the domain method, but in this case, the computation must be performed throughout the domain, which requires a much higher computational cost than the boundary method. For continuum-based shape DSA using the boundary method, the IGA provides more accurate values than the conventional FEA; The FEA-based boundary method provides erroneous results due to the inaccurate consideration of the boundary geometry such as normal vector and curvature, while the IGA-based one accurately considers the geometry of boundary. The required computational cost for the boundary method is much less than that of the domain method since the computation is performed only on the boundary.

The shape sensitivity of performance measure defined by a boundary functional on the non-smooth boundary can be precisely obtained using the curvature of boundary, the normal component of design velocity, and the tangential divergence of design velocity [3]. Especially for problems with non-smooth boundaries, the tangential divergence must be considered, but it is not possible to calculate it accurately with conventional FEA-based boundary method. Through numerical examples, the accuracy and efficiency of the IGA-based boundary method for DSA are compared with other methods such as FEA-based boundary and domain methods. It is demonstrated that the IGA-based shape design sensitivity of the boundary functional could accurately represent the tangential divergence on the boundary that the linear shape function in the FEA-based one cannot properly represent.

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Quantum scientific computing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GROUND ENERGY AND RELATED PROPERTIES ESTIMATION IN QUANTUM CHEMISTRY WITH LINEAR DEPENDENCE ON THE NUMBER OF ATOMS

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ABSTRACT

Density-functional theory (DFT), due to its ability to predict ground state properties without explicitly solving a many-body quantum mechanical model, has revolutionized computer simulations in chemistry and material science. A faithful implementation of the theory requires self-consistent calculations, involving repeatedly diagonalizing the Hamiltonian, for which a classical algorithm typically requires a computational complexity that scales cubically with respect to the number of electrons. This limits DFT's applicability to large-scale problems with complex chemical environments and microstructures. In this talk, we present a quantum algorithm that has a linear scaling with respect to the number of atoms, offering a drastic reduction in computational cost. Our algorithm leverages the quantum singular value transformation (QSVT) (András Gilyén et al, 2019) and an unbiased amplitude amplification method (Patrick Rall and Bryce Fuller, 2023) in order to generate a quantum circuit that encodes the density-matrix, and estimate the output electron density with the Heisenberg-limited scaling. We present an efficient hybrid approach to accelerate the self-consistent field calculations by reducing the number of components of the electron density that need to be estimated by quantum computation. We provide a rigorous convergence analysis that involves the function approximation error, the statistical fluctuation, and the iteration complexity.

Architected materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFICIENT TWO-SCALE MODELING OF NONLINEAR HYPERELASTIC STRUCTURES AND ARCHITECTED MATERIALS

Dennis Kochmann[*1], Helen Le Clezio*[1], Claire Lestringant*[2] and Konstantinos Karapiperis*[1]

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ABSTRACT

We present a numerical framework for modeling truss-based architected materials, which accounts for both the geometric nonlinearity inherent in the large deformation of slender struts and the nonlinear constitutive behavior of hyperelastic base materials. Akin to the FE2 method in homogenization, our approach is based on a formal, two-scale expansion. We decompose the 3D description of a structure into a macroscale problem (solving for the deformation of all beam center-lines, taking into account stretching, bending, and torsion) and a series of microscale boundary value problems defined over the beam's cross-section. To bypass the expensive pre- or on-the-fly solution of the cross-sectional problem on the microscale, we use machine learning to learn a surrogate for the effective energy density of the microscale problem, which is subsequently used in the macroscale problem based on a geometrically exact, nonlinear discrete beam framework. We demonstrate the accuracy of this approach through a set of benchmarks, highlighting the nonlinear effects of the cross-sectional geometry and constitutive material, including material heterogeneity and pre-strains. We further illustrate its application to truss-based architected materials consisting of networks of slender polymeric beams.

Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELLING FOR 4D PRINTING OF PHASE TRANSFORMING CELLULAR MECHANICAL METAMATERIAL

Sosuke Kanegae[1], Hayato Nagayama[1], Saki Morimoto[1], Masayuki Okugawa[1] and Yuichiro Koizumi[1]*

[1]Osaka University

ABSTRACT

Mechanical metamaterials have undergone revolutionary development due to additive manufacturing (AM) technologies, represented by authentic materials with negative Poisson ratios. On the other hand, AM technology of 3D objects that evolve in shape over time and in response to environmental change is emerging as 4D printing technologists, as represented by Phase Transforming Cellular Materials (PXCM) for various applications. We are developing PXCMs that exhibit phase transformations in crystalline materials induced by stress or temperature change, as in shape memory and superelastic alloys. We propose a novel design for mechanical metamaterials with temperature- and stress-responsive stable structures, offering the potential to apply to large-scale constructions with shape memory and superelastic capabilities. This innovation is anticipated to provide earthquake- resilience through advanced shock absorption and seismic isolation technologies.

Our approach encompasses three pivotal aspects:
1. Multi-Axed Stress-Induced PXCM: We designed a lattice structure based on face-centered cubic atomic arrangements, capable of phase transitions under stress along four <111> directions. The lattices consist of spherical nodes connected by beams aligned in the <110> direction, akin to atomic bonds. These beams are shaped similarly to curly brackets and undergo significant deformation via buckling under a stress beyond a stress threshold, providing impact absorption. The metamaterial's behaviors were analyzed by Finite Element Method (FEM) and predicted by machine learning with neural networks. The model was validated by actual fabrication using polyurethane with Powder Bed Fusion.
2. Thermally-Induced PXCM: We fabricated PXCMs to demonstrate thermally induced phase transitions utilizing bimetallic (Fe-36Ni Invar and Mn-Cu alloys) beams. The design incorporates beams that exhibit phase changes unidirectionally under load. The FEM model was used to construct a phase diagram indicating the stabilities of phases in stress-temperature space. The model was verified by constructing a 2D PXCM, which exhibited stress- and thermally-induced phase transformations.
3. Multi-Material 3D Printing for 4D Applications: The creation of PXCMs with thermal phase transformation necessitates multi-material AM techniques. In powder-based AM technologies, such as Directed Energy Deposition (DED), Binder Jetting, and Powder Bed Fusion (PBF), important issues are separating, collecting, and recycling mixed powders. We developed a novel vibratory process for powder separation experimentally. The factors influencing the separation efficiency were analyzed through discrete element method (DEM) simulations.

This study contributes to the development of mechanical metamaterials in disaster mitigation infrastructure and extends the possibility of the functional metamaterial fabricated by AM.

Deep and machine learning methodology in the context of application to computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREDICTION OF THREE-DIMENSIONAL DEFECT'S INFORMATION IN COMPLEX SHAPED CFRP SPECIMENS USING GNN BASED ON STRESS DISTRIBUTION ON SURFACE FROM HOMOGENIZED FINITE ELEMENT ANALYSIS AND INFRARED MEASUREMENTS

Yuta Kojima[*1], Kenta Hirayama[1], Yoshihisa Harada[2] and Mayu Muramatsu[1]*

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ABSTRACT

In this study, a machine learning model which is pretrained by the distribution of sum of the principal stress on surface (DSPSS) obtained from simulations by the finite element method (FEM) is used to predict three-dimensional information of defects from DSPSS obtained from infrared stress measurements for the complex shaped carbon fiber reinforced plastic (CFRP). The complex shaped CFRP used in this study is a children's athletic prosthetic leg that has both curved and straight geometries. Generally, CFRP structures are made by laminating prepregs with different microstructures. The model prepared in this study is laminated with a combination of plain weave structure and unidirectional structure. The plain weave structure is used in the prepregs which are located near the surface. Infrared stress measurements are performed to obtain DSPSS calculated from surface temperature changes using Kelvin's theory of thermoelasticity. In experiment, the bolted joints are fully fixed, and loads are applied to the surface which is in contact with the ground. The measured surfaces are painted black to prevent surface reflection. Measurements are performed on 4 specimens without defect and 16 specimens with defect. A homogenized FEM is used to obtain DSPSS which is close to the stress distribution of the infrared stress measurement. It performs a macro-scale analysis that takes into account the mechanical properties of the microstructure of the plain weave structure and unidirectional structure. As in the infrared stress measurement, the bolted joints are fully fixed and a load is applied to the surface which is in contact with the ground. The used mesh is a four-node tetra element. Analysis is performed on a specimen without defect and a specimen with defect. The machine learning model used in this study is a graph neural network (GNN), which can be trained with nodes and edges in a three-dimensional geometry and can therefore make good predictions for objects with curved surfaces, such as the prosthetic leg. Firstly, the GNN model is pre-trained using DSPSS obtained from FEM, for which a large number of data sets can be prepared. Next, we perform transfer learning using DSPSS obtained from infrared stress measurements, for which only a small amount of data set is available, to estimate the three-dimensional information of the defects with high accuracy.

Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FATIGUE LIFE PREDICTION WITH ELASTO-PLASTIC DAMAGE AND HARDENING MODELING

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ABSTRACT

This contribution introduces an innovative and efficient methodology for modeling fatigue induced by damage, emphasizing speed and robustness. The proposed approach utilizes a rate-dependent elasto-plastic gradient-enhanced model, offering a comprehensive solution for capturing material degradation over time. The theoretical foundation of the model is established through an extended Hamilton principle for dissipative processes, incorporating internal variables as damage, elasto-plasticity and hardening.

To mitigate mesh dependency issues, the Helmholtz free energy is enhanced by gradient terms for regularization purposes. This adjustment allows for the effective fitting of fatigue models to experimental data, primarily facilitated by the fatigue rate parameter, enabling a precise characterization of material deterioration.

Efficient resolution of the coupled system of equations is achieved through an operator split and the application of the Neighbored Element Method. This integrated approach not only enhances the accuracy of the fatigue model but also significantly improves computational efficiency. By doing so, it establishes a robust framework for comprehending and addressing the intricate challenges associated with fatigue-induced damage in engineering applications.

The methodology's strength lies in its ability to balance the intricacies of fatigue modeling with the need for computational efficiency. The operator split technique streamlines the solution process, while the Neighbor Element Method contributes to the overall effectiveness of the coupled system.

Keywords: Damage, Fatigue, Gradient-enhanced regularization, Neighbored element method, Coupled processes, Variational modeling

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Computational fluid dynamics (CFD) and fluid-structure interaction (CFSI): Methods and Applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOWARDS ROBUST IMMERSED INTERFACE FLUID-STRUCTURE INTERACTION ALGORITHMS FOR COMPLEX GEOMETRIES

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ABSTRACT

In this talk, we present ongoing work on the development of accurate and efficient numerical methods for fluid-structure interaction. Our approach is based on a recently developed immersed interface method for discrete surfaces, avoiding the use of body-conforming discretizations for the moving fluid-structure interface. We employ a structured discretization of the fluid equations combined with a Lagrangian discretization of the structural dynamics in a partitioned algorithm. Kinematic matching conditions are imposed as a constraint on the motion, enforced through a Lagrange multiplier force along the fluid-structure interface. This numerical approach integrates stress jump conditions generated by the surface force within the Cartesian discretization, allowing us to capture accurate fluid traction forces up to the fluid-structure interface. The basic method is extended to handle both rigid-body and flexible-body fluid-structure interaction using a simple Dirichlet-Neumann coupling scheme. Numerical tests indicate that the method avoids artificial added mass instabilities. The talk will delve into the details of the numerical methodology and its extensions, addressing irregular interface discretizations that may arise in models involving complex geometries and at contact or near-contact conditions. The methodology will also be illustrated through selected biomedical applications.

MFEM: ACCELERATING EFFICIENT SOLUTION OF PDES AT EXASCALE

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ABSTRACT

Modern GPU architectures favor algorithms that expose fine-grain parallelism and maximize the ratio of floating-point operations to energy intensive data movement. One of the few viable approaches to achieve high efficiency in the area of PDE discretizations on unstructured grids is to use matrix-free/partially-assembled high-order finite element methods, since these methods can increase the accuracy and lower the computational time due to reduced data motion.

In this talk we present an overview of MFEM (https://mfem.org), a library for scalable high-order finite element methods, which powers high-performance computing applications in a wide variety of fields. We also report on the body of work in the Center for Efficient Exascale Discretizations (https://ceed.exascaleproject.org/), which was a co-design center in the US Exascale Computing Project focused on next-generation discretization software and algorithms, where MFEM plays a major role.

Our approach to efficiency is based on a "matrix-free" representation of the finite element operator, that factors a bilinear form into a series of sparse and dense components corresponding to the parallelism, mesh topology, basis, geometry, and pointwise physics in the problem. The operator decomposition exposes several layers of parallelism, enables the use of batched dgemss and tensor contractions, and only requires quadrature point values to be assembled for computing the action. This "partial assembly" formulation results both in less (nearly optimal) computation and less (optimal) data movement compared to assembling a global sparse matrix, therefore increasing performance and reducing time to solution.

We will describe recent MFEM advancements in performance optimizations for GPU architectures, high-order finite element benchmarks and miniapps, scalable unstructured adaptive mesh refinement, matrix-free preconditioning for partially assembled operators, high-order data analysis and visualization, and demonstrate their impact in several large-scale applications from the US Department of Energy.

Advanced multiscale and adaptive numerical methods for non-linear solids
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AUTOMATIC MULTILEVEL MESH REFINEMENT FORMALISM FOR LINEAR AND NONLINEAR SOLID MECHANICS

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ABSTRACT

This study provides a comprehensive investigation of Adaptive Mesh Refinement (AMR) methods within a generic algorithmic framework. We propose a fully-automatic mesh refinement framework driven by an a posteriori error estimator facilitating an on-the-fly refinement. The adopted AMR mechanism is based on user-prescribed tolerances on errors guaranteeing simulation results meeting predefined accuracy standards.

First, we compare the adaptive multilevel Local Defect Correction (LDC) method [1] to hierarchical (conforming and non-conforming) h-adaptive refinement techniques in the context of linear elastic solid mechanics. We provide a numerical assessment of their performances for all-quadrilateral and all-hexahedral meshes within the developed AMR framework. Our results demonstrate the superior efficiency of the multilevel LDC method, highlighting its great potential in solving implicit systems in elastostatic simulations based on standard metrics of efficiency (dimension of systems to be solved, storage requirements, CPU time) [2]. Due to its versatile nature, this method is able to accommodate different solvers, material models, and meshes on different levels, eliminates the necessity for a complete remeshing of the domain, and benefits from a non-intrusive implementation.

We further extend the adopted computational framework to the nonlinear quasi-static solid mechanics context, aiming to capture the evolution of multiscale phenomena over time [3]. It centers around the multilevel LDC method, which, in addition to its attractive properties mentioned above, showcases its inherent capability to dynamically generate refined mesh hierarchies that capture the evolving phenomena over time.

In the nonlinear context, the proposed AMR framework manages fields transfer between different time steps and non-matching meshes and maintains error control over time through an efficient equilibration strategy. Moreover, it encompasses a reliable remeshing algorithm which minimizes mesh regeneration frequency over time, ensuring compliance with prescribed tolerances and optimizing computational resources. Effectiveness and robustness of the proposed algorithm are validated through diverse 2D and 3D numerical experiments involving various material behaviors and loadings.

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Model order reduction for parametrized continuum mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTILINEAR SUBSPACES WITH TENSOR DECOMPOSITIONS FOR PROJECTION-BASED REDUCED ORDER MODELLING

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ABSTRACT

A widely used technique for data-driven model order reduction is projecting onto an orthogonal subspace discovered using truncated singular value decomposition (SVD). In practice, applying SVD requires converting the training data into a matrix, which concatenates modes that are otherwise independent (e.g., X/Y/Z spatial coordinates, variables) and obscures interactions among the independent modes that could be leveraged for efficient and accurate dimensionality reduction. We propose a multilinear alternative, using tensor decompositions, to discover a subspace that is distinct along the independent modes and provides a much better trade-off between accuracy and dimensionality reduction than matrix SVD. Tensor decompositions are higher-order extensions of matrix factorizations and, specifically, higher-order SVD (HOSVD) is a proper generalization of matrix SVD to higher dimensions.

We present techniques of applying truncated HOSVD that allows discovering separate subspaces along the independent modes of high-dimensional data. The resulting subspaces are interpretable, with precise control of a target rank along each mode of the high-dimensional data tensor. Moreover, for a specified overall 2-norm error, HOSVD allows flexibility in partitioning the truncation error along the independent modes that can prioritize accuracy of some mode(s) over other. The individual subspaces are compact, and the effective subspace of the concatenated dimensions is related to tensor product of the individual bases.

We apply the truncated HOSVD based dimensionality reduction to a climate dataset representing the atmospheric dispersion of a volcano eruption. The dataset comprises atmosphere ensemble model predictions of a simulated volcano eruption, at various forcing strengths of the volcano and different initializations of the turbulent flow field. Dimensionality reduction is sought specifically for the combined spatial modes (latitude, longitude) and multiple variables in the dataset. We compare SVD applied to the matricized data (latitude, longitude, and variables concatenated into a single dimension) with truncated HOSVD applied to the data in its original tensor form. We demonstrate that, for the same target 2-norm truncation error, HOSVD results in better accuracy in predicting unseen (test data) snapshots. We discuss how the multilinear model can be extended for other downstream tasks, e.g. training a surrogate flow map in the combined subspace using DNNs, by retaining the tensor product structure between the individual mode subspaces.

Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DETERMINATION OF OPTIMAL BEAM SHAPES IN LASER POWDER BASED FUSION OF METALS

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ABSTRACT

We present a framework for laser beam shaping in L-PBF/M that uses an advection-diffusion model to compute a laser intensity profile corresponding to a desired temperature field (i.e. melt pool shape)[1]. To solve this inverse problem, we minimize the functional given by the squared difference between the predicted and the desired temperature field integrated over the domain using the adjoint-based optimization method. The melt pool dimensions produced by the computed laser intensity profile are validated using photomicrographs of experiments. However, other quantities such as temperature profiles, temperature gradients, or dynamic effects cannot be validated experimentally. To this end, the computational results are compared to high-fidelity melt pool models (using Smoothed Particle Hydrodynamics). Additionally, we will present new types of laser intensity profiles designed to achieve a wide, shallow, yet stable melt pool in conduction mode.

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Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MIXED FINITE ELEMENT APPROACH FOR THERMO-PORO-ELASTO-PLASTIC SIMULATION OF STIMULATED VOLUME EVOLUTION IN SUBSURFACE APPLICATIONS

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ABSTRACT

A new mixed nonlocal finite element framework is developed for nonlinear thermo-poro-elasto-plastic simulation of porous media with multiphase pore fluid flow and thermal coupling. The solid-fluid interaction is accounted for using the mixture theory of Biot based on the volume fractions concept. Different sources of nonlinearities arising from the multiphase fluid flow effects, advective-diffusive heat transfer, inelastic deformation, fluid flux injection induced mechanical tractions, solid skeleton deformation permeability dependence, and temperature dependent viscosity are included in developing a robust numerical solver for the targeted coupled multi-physics problem. To address the effect of microstructure in inelastic localized deformation behaviour with dilational softening, a nonlocal plasticity model is proposed based on a characteristic length scale which rectifies the non-physical pathological mesh dependence problem encountered in conventional plasticity. The accuracy and strength of the developed model is shown with comparing the obtained numerical results of a benchmark bilateral compression test with existing published data in the literature. To show the versatility and robustness of the developed computational framework in modelling the geomechanics of real-case engineering practices, large scale thermo-hydro-mechanical (THM) subsurface stimulation processes with applications in Enhanced Oil Recovery (EOR) are effectively simulated and the targeted enhanced recovery and performances are demonstrated. The current formulation does not include phase transformation modelling capability, and therefore, the developed models may not be applicable for simulation of the engineering processes that involve phase change behaviour (e.g., steam injection).

Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREDICTING DUCTILE FRACTURE DURING TORSION TESTING USING DISLOCATION DENSITY TENSOR

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ABSTRACT

A model based on dislocation density tensor [1] is proposed for predicting ductile fracture during torsion testing. The effect of prestrain bestowed by bar drawing on the fracture strain is examined. First, a simple torsion testing machine, which can be incorporated into a universal testing machine, is manufactured. Since the cross-sectional shape of the specimen is uniform and circular along the length owing to bar drawing prior to torsion testing, the upper and lower chucks which clamp the specimen are contrived. Next, a method for simulating the torsion testing of a bar is proposed using a periodic boundary condition, and is proved to be effective for reducing the calculation time drastically. The fracture strain calculated using the dislocation density tensor-based model agrees with the experimental values, whereas the fracture strain calculated using the ellipsoidal void model proposed previously [2] does not agree with the experimental values. Finally, the fracture strain calculated using the previously proposed practical model based on the consideration ratio of prestrain [3] agrees with the experimental values.

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CAHN-HILLIARD-TYPE DIFFUSION COUPLED WITH ELASTICITY

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ABSTRACT

The Cahn-Hilliard equation is a nonlinear parabolic equation of fourth order, which characterizes diffusion by considering the gradient in chemical potential, rather than following classical Fickian diffusion. The fourth order term in the equation necessitates the usage of C1 approximation requiring interelement continuity of the primary variables (concentration) and their derivatives. In this study, we introduce a phase field algorithm that couples the Cahn-Hilliard equation with the equation of linear elasticity, with a focus on computational aspects. We propose a staggered algorithm to solve the two equations, using the Natural Neighbor Galerkin method (also called the Natural Element Method) to generate shape functions via Voronoi diagram and Delaunay triangulation. We use C1 NEM shape functions to compute concentration and C0 NEM shape functions to compute displacements. An iterative solver with the Newton-Raphson method is employed to solve the set of equations. The elasticity effects due to microstructure evolution by employing the concept of eigenstrains and investigate the effect of eigenstrains on microstructural evolution of an inclusion in a 1×1 square domain is studied. Finally, we simulate the behavior of two inclusions, with and without applied displacements. When two inclusions are present, a variation in the equilibrium configuration can be observed between the conditions of applied external displacement and the absence of such displacement. Mixed approach for Cahn-Hilliard equation is studied and implementation is carried out in Abaqus with the help of user subroutines. The elasticity effects are studied in detail with the help of several parametric studies.

Numerical modeling of granular and multiphase flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SPEEDING UP CALCULATION TIME BY SPECIFYING SEARCH RANGE IN SQUEEZE COMPACTING ANALYSIS USING DISCRETE ELEMENTS WITH PARTICLE SIZE DISTRIBUTION

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ABSTRACT

Discrete Element Method (DEM) is a numerical method used to simulate dynamic phenomena of granular materials such as sand. There is a speeding up method of calculation time using neighboring particle search in DEM with uniform particle size [1]. However, to reduce computational cost while keeping calculation accuracy, it is necessary to determine the specified search range and its update interval.

In the foundry engineering field, various CAE software are used to simulate phenomena such as mold filling, heat transfer, and solidification. However, since green molding sand is a discontinuous material, the development of mold-making simulations has been delayed. Y. Maeda et. al. [2,3] have proposed the green sand modeling called the Hard-Core/Soft-Shell model, which takes into consideration the characteristics of green sand with particle size distribution and cohesion. Further, the identification method from a real particle size distribution to the discrete element has been proposed and it indicated the usefulness of molding simulation using DEM. However, DEM using discrete elements with particle size distribution requires a huge amount of calculation time.

In this study, we try to speed up calculation time by neighboring particle search in squeeze compacting analysis using discrete elements with particle size distribution. How to determine the time step, the specifying search range and the update interval of it are investigated. From the simulation results, the appropriate conditions in the case with particle size distribution are different from those in the case with uniform particle size, and it is necessary to take into consideration the size and the ratio of a peak in the particle size distribution map. Because it is greatly influenced by particle size distribution, it is clarified it has better use a large and a small search range determined by its particle size. The calculation speed is improved for any particle size distribution within the condition for the present study.

Keywords: Discrete Element Method, Squeeze compacting, Particle size distribution, Search range

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Mesh-free particle methods for multi-physics problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NON-NEWTONIAN MODEL FOR SIMULATING SAND FLOW WITH MOVING PARTICLE HYDRODYNAMICS (MPH) METHOD

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ABSTRACT

Sand flow simulation was conducted by extending the moving particle hydrodynamics (MPH) method [1-4]. Specifically, the Mohr-Coulomb yield criterion was introduced in the Bingham model [5]. With this non-Newtonian model, the sand flow behavior was reproduced. The variation of the angle of repose when the sand collapse was well expressed by varying the internal friction angle of the Mohr-Coulomb model.

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Imaging-based methods in computational medicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AUTOMATED MESH CONSTRUCTION FROM IMAGES FOR CARDIAC SIMULATIONS IN PATIENTS WITH CONGENITAL HEART DEFECTS

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ABSTRACT

Congenital heart defects (CHDs) are characterized by abnormal cardiac anatomies that dramatically impact patient outcomes. Personalized computer heart models derived from patient image data can facilitate personalized treatment planning of CHDs and surgical/procedural decision-making. However, prior studies often require prohibitively laborious human efforts to generate models from patient images. Prior deep learning (DL) methods demonstrated potential in automating cardiac reconstruction but are mostly designed to model normal cardiac structures(1). Therefore, we aim to develop a DL algorithm to generate cardiac models automatically from CHD patient images to support cardiac mechanics simulations.

Our algorithm leverages both the CHD diagnosis (types of CHD) and image data to construct cardiac models from CT images. We use neural networks (NNs) to approximate signed distance functions (SDFs) that represent the CHD anatomical abnormalities given the input diagnosis. Our method then deforms these type-specific SDFs to match target patient images. To preserve the cardiac anatomies learned by the type-specific network, we leverage neural ordinary differential equations (NODE) to learn the diffeomorphic mapping between the learned type-specific geometries (type space) and patient-specific cardiac geometries (shape space). Namely, we learn the motion of points from the shape space to the type space based on the image data. To incorporate patient image data into the NODE, we use a convolutional NN to extract an image feature volume from which we sample the image feature vectors at points in the shape space.

We used a total of 108 CT images (67 for training, 4 for validation, and 37 for testing) that covered cases of ventricular septal defects (VSD), atrial septal defects (ASD), Tetralogy of Fallot (ToF), transposition of great arteries (TGA), double outlet right ventricle (DORV) and pulmonary atresia (PuA), respectively. Our networks were successfully trained to predict type-specific SDFs that captured the typical abnormalities given the input CHD type. When evaluated on testing images, our method constructed cardiac anatomies consistent with the input CHD diagnosis, whereas the prior segmentation approach, UNet(2), produced many topological artifacts. To construct simulation-ready meshes, we created simulation-ready meshes at the type space and used our trained DL algorithm to deform the corresponding template to match with patient images. Ongoing work includes creating meshes for a cohort of DORV patients to conduct computational fluid dynamics simulations, which can reveal detailed flow patterns for individual patients to assist surgical planning.

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Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STUDY ON PERFORMANCE AND HYDRAULIC LOSSES OF CENTRIFUGAL PUMPS WITH IMPELLERS HAVING POROUS STRUCTURE

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ABSTRACT

The impeller of a centrifugal pump must have a structure that can be used stably over a wide flow range and that allows operation with high pump efficiency even at low-flow-rate and high-head. In this study, a closed impeller with a porous structure with radial and annular flow channels was proposed, which is expected to be effective in suppressing vortices generated inside the channels, which hinder low-flow-rate and stability, by a design that does not narrow the blade width and narrows the flow channels. The authors undertook experiments and simulations to elucidate the performance of pumps using that impeller and to accurately predict its performance.

In the experiment, the pump performance was measured with an impeller fabricated by a 3D printer. The results showed stable operation over a wide-flow-range and characteristics that prevent the pump efficiency from decreasing even in the high-flow-range.

In the simulation, a loss analysis method using unsteady CFD results was proposed to investigate the variation of internal flow and various hydraulic losses during one rotation of the impeller. As a result, it was elucidated that the increase in total hydraulic losses of the pump with increasing flow rate is due to losses in the impeller other than friction losses due to changes in the size of the vortex in the impeller. Furthermore, it was elucidated that the variation of total head with impeller rotation is affected by losses in the volute casing other than friction losses originating from the vortex generated by the rear shroud and intermediate disk near the outlet of the radial flow channels.

Based on these results, an impeller with a porous structure is useful for centrifugal pump applications. CFD using the Navier-Stokes equations as the basic equations and SST as the turbulence model is effective for the analysis of this impeller. Furthermore, the loss analysis method using CFD results is expected to assist in the development of this type of impeller, since the losses could be evaluated quantitatively.

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NONLINEAR MULTILEVEL AND DOMAIN DECOMPOSITION METHODS FOR PHASE-FIELD FRACTURE SIMULATIONS

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ABSTRACT

The numerical simulation of failure mechanism in solids is computationally challenging, as crack paths with a possibly complex topology have to be resolved. Phase-field approach for fracture simplifies and overcomes these difficulties by regularizing the sharp crack interfaces by means of a diffusive damage model. The main challenge associated with phase-field fracture modeling is that it requires a solution of a strongly nonlinear coupled system of equations at each loading-step. This is computationally demanding due to the non-convexity of the coupled energy functional and a large number of degrees of freedom required to resolve the damaged zones. In this work, we propose to solve the arising nonlinear problems efficiently using nonlinear multilevel and domain decomposition methods. The proposed methods are designed to solve the arising non-linear problems in a monolithic manner by taking advantage of the underlying structure of the coupled problem. More precisely, we demonstrate how to construct a hierarchy of suitable sub-spaces, related to different levels or subdomains. In the multilevel settings, we employ level-dependent objective functions, that combine a fine-level description of the crack paths with the coarse level discretization. In the domain decomposition settings, we construct a preconditioner for inexact Newton's method by partitioning the degrees of freedom into two sets, related to the displacement and the phase-field. We will demonstrate the convergence behavior of the proposed multilevel and domain decomposition methods using standard benchmark problems. A comparison with the widely-used alternate minimization scheme will be also presented, showing a significant reduction in the number of iterations as well as in the execution time.

COMBINING SPACE-FILLING CURVES WITH HYBRID PARALLELIZATION FOR EFFICIENT IN-MEMORY LOAD BALANCING

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ABSTRACT

Particle-laden turbulent flows occur in a wide range of engineering application such as spray injection, wind energy and turbomachinery. The numerical domains required for these applications can often only be discretized using unstructured meshes. While facilitating grid generation, parallelization of particle tracking algorithms on these grids is challenging as particles can cross several numerical elements during a single time step with their trajectories are only weakly correlated to the fluid phase. The present talk presents a hybrid parallelization strategy developed for the high-order massively parallel Discontinuous Galerkin Spectral Element Method (DGSEM) framework FLEXI[1,2]. The challenge of non-local particle tracking is addressed using halo regions, which enrich the local domain with geometric information up to a certain physical distance from the domain boundaries. Using the MPI-3 shared memory model in combination with space-filling curves, geometric information is assigned either to processor-exclusive memory regions or made accessible on a compute node level[3]. Utilizing remote memory access and hardware offloading, the method is applied to in-memory load balancing. Here, runtime information such as field information and particle positions are dynamically redistributed before the simulation is seamlessly continued. Special care is taken to optimize re-initialization times while minimizing communication load on the interconnect. This work concludes by presenting examples of large scale computations of particle-laden turbulent flows in complex systems and giving an outlook on the next research challenges.

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Virtual elements for partial differential equations on polytopal meshes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AUTOMATION OF HIGHER ORDER VIRTUAL ELEMENT METHODS

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ABSTRACT

The paper deals with the computational efficiency and simplicity of implementation of nonlinear higher-order virtual elements. When compared to the standard FEM the VEM lacks the simplicity of derivation of formulae and simplicity of computer implementation. This becomes especially problematic with an increasing number of polygon or polyhedral vertices, an increasing VEM order, and especially for the 3D problems. The paper presents an improved ADB (automatic differentiation based) formulation of VEM combined with an automatic derivation of corresponding formulae and automatic generation of computer code using AceGen automatic code generation system. When applied to nonlinear, path-dependent, coupled problems, such as finite strain plasticity, computational efficiency regarding the evaluation of the element tangent matrix and residual can also pose a problem. Already for a second-order, three-dimensional VEM, implementation of a complex nonlinear model can pose a significant problem, and mostly only low-order implementations have been reported in the literature so far. The paper employs a fast quadrature compression based on the computation of discrete Leja points by LU factorization (Sudhakar 2017) that, for a given accuracy goal, reduces the high number of integration points that emanate from the braking of an arbitrary polyhedral into a union of tetrahedrons. The discrete Leja points can be calculated for an arbitrarily shaped polyhedron thus enabling an efficient integration of consistency part of the VEM tangent matrix and residual. The use of FEM stabilization is essential for the convergence of highly nonlinear problems; however, its evaluation can also be computationally expensive. The computational cost of the stabilization matrix can be reduced by exploiting the sparsity structure of the resulting stabilization matrix at the individual VEM level.

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Numerical modelling of composite materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STOCHASTIC FE-BE METHOD FOR HOMOGENIZATION ANALYSIS OF 2D DIFFUSION PROBLEMS CONSIDERING UNCERTAINTIES OF INCLUSION SHAPE

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ABSTRACT

The stochastic method for homogenization analysis of diffusion problems considering uncertainties of inclusion shape is developed using a microscopic stochastic BEM and a macroscopic FEM. The spatial variation of inclusion shape is modeled using Karhunen-Loeve expansion with exponential-type covariance kernels. The characteristic function on a 2-D unit cell and the homogenized diffusion tensor are calculated using the stochastic BEM. The macroscale diffusion problems are solved using the stochastic FEM with the polynomial chaos (PC) expansion. Through numerical tests, the expected value and the standard deviation of the concentration in a macroscale problems and their distribution are investigated.

Extended digital twins including uncertainty and complexity of human/society and human knowledge
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE ROLE OF HUMANS IN COMPUTATIONAL MECHANICS – VERIFICATION AND VALIDATION FOR QUALITY MANAGEMENT –

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ABSTRACT

Verification and Validation (V&V) for quality management describes the role of humans in manufacturing industry from the technical viewpoint. A typical document of V&V for quality management is ISO9001 [1]. The documents of V&V for computer simulation have been published as [2, 3]. They include additional requirements specific for computer simulation as well as the general requirements in ISO9001. A typical procedure satisfying the requirements for computer simulation is provided in [4] and examples are shown in [5]. V&V for quality management is derived from our experiences of human activities in manufacturing industry to enhance the credibility of the products.

Competence required in the V&V for quality management is related to the education. For example, a qualification system for the specialists is recommended to be fair and transparent treatment of competence. Japan Society of Mechanical Engineers (JSME) manages a qualification system for computational mechanics for about 20 years [6]. Competence of humans involving the knowledge of computational mechanics should be kept high as well as detailed procedures and documents are required in the quality management system.

V&V for modeling and simulation [7] is another type of V&V for computational mechanics. Both V&Vs for quality management and modeling and simulation are needed.

Society5.0 is a concept of future society envisaged by the Government of Japan [8]. Utilization of digital twins is aimed for future industries where humans should be placed in the center of the society. There are two types of the humans considered in Society5.0: working people and customers. In the past, working people are expected to be accurate and efficient and the quality management system has been used for this purpose. In future, well-being of working people is more important and has to be included in the quality management system.

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Space-time modeling of coupled problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GOAL ORIENTED ERROR ESTIMATION FOR SPACE-TIME ADAPTIVITY IN PHASE-FIELD FRACTURE

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ABSTRACT

In this talk, we introduce a phase-field fracture model in a space-time formulation and use the dual-weighted residual (DWR) method to formulate a goal oriented error estimator for adaptive refinement in space and time. Tensor-product space-time finite elements are being used with continuous elements in space and discontinuous elements in time, such that the primal problem can be solved with a time-stepping scheme. The temporal derivative of the phase-field variable is added as a regularization term in the Euler-Lagrange equations to allow for backwards time-stepping in the dual problem. The error is localized using partition of unity (PU). The convergence order of the space-time adaptivity is analyzed on numerical tests with different goal functionals.

Verification techniques in computational physics and applied mathematics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFECT OF MATHEMATICAL MODEL SIMPLIFICATIONS ON SOLUTION VERIFICATION EXERCISES

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ABSTRACT

The quantification of the numerical uncertainty of simulations through solution verification exercises is imperative to evaluate the accuracy of the results and make predictions, i.e., computations with a quantified and adequate degree of uncertainty that can be confidently used in engineering projects, even if reference data is unavailable or scarce. Accuracy assessments are particularly relevant to transient multi-material mixing flows due to i) complex multi-physics, ii) transient nature that makes computational errors behave nonlinearly and cumulatively, iii) most solution verification methods not being tested on such problems, and iv) common mathematical model assumptions and simplifications. The Euler equations (EE) are an example of a simplified mathematical model widely used in transient multi-material mixing problems featuring shock waves and high-Mach number flow (e.g., stellar astrophysics, shock-driven mixing, and high-speed combustion). It simplifies the Navier-Stokes equations (NSE) by assuming adiabatic and inviscid flow, i.e., neglecting heat conduction, viscous, and diffusivity effects. Despite the importance of the EE, the continuous enhancement of computing power and numerical methods makes assessing the envelope of such a mathematical model crucial. For example, neglecting the molecular viscosity makes the effective Reynolds number of simulations solely determined by the numerical viscosity and assumes an “infinite” Reynolds number. However, how high of a Re is high enough? What is the impact of an effective Re uniquely determined by the numerical viscosity on solution verification?

This work evaluates the impact of the EE on solution verification exercises of transient multi-material mixing flow simulations. Toward this end, we simulate four flows with the EE and NSE: i) 1D Riemann problem, ii) 2D triple point problem, iii) 3D Taylor Green Vortex, and iv) 3D Richtmyer-Meshkov multi-material flow measured at LANL. The computations are performed on several mesh/time resolutions to evaluate their dependence on this parameter and estimate the numerical uncertainty. From a validation point of view, the results show that inviscid and adiabatic assumptions strongly impact the simulations' physics, hampering comparisons between simulations and reference data. This outcome stems from the inability to bind the effective Re and consider heat conduction. Such assumptions can also impact solution verification exercises by significantly increasing the cost of converging the simulations upon grid refinement and artificially increasing the numerical uncertainty and the cost of solution verification exercises. Overall, the results indicate that modeling assumptions strongly impact not only validation exercises but also solution verification.

Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATION OF THE MATERIAL POINT METHOD IN METAL CUTTING SIMULATIONS UTILIZING THE JOHNSON-COOK MATERIAL LAW

Marvin Koßler[1], Sascha Maassen[1], Rainer Niekamp[1] and Jörg Schröder[1]*

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ABSTRACT

The Material Point Method provides an alternate method for simulations, differing from traditional techniques like the Finite Element Method (FEM). This method utilizes material points for body discretization, with the equations' solutions being executed on a computational background grid, see e.g. [1]. The simulation process during a single time step involves three primary steps. Initially, kinematic quantities of the material points are transferred to the grid nodes. Once gathered, the solution is determined at the grid nodes and then reassigned back to the material points, followed by updating their position, velocity, stress, and deformation state individually. For subsequent time steps, the existing grid is discarded in favor of a new one since it holds no persistent information. This approach allows the material points to move independently from the background grid, thus preventing mesh distortion in cases of huge deformations, a problem sometimes encountered in FEM simulations. This contribution presents simulations of three-dimensional metal cutting in both vertical and horizontal orientations. These simulations utilize the Johnson-Cook material law, see [2], which accounts for plastic strain rates and heat generated from plastic deformations. Additionally, the grid-shift method is employed to enhance solution smoothness as recommended in [3].

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ON SOLVING CONTACT PROBLEMS USING SUBSTRUCTURING DOMAIN DECOMPOSITION METHOD

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ABSTRACT

Contact problems refer to modeling of the interaction between two or more elastic bodies when they are in contact with each other. While solving such contact problems, we must accurately model the forces the bodies induce at the contact surfaces and compute the resultant deformation due to the interaction between bodies. These problems are common in many scientific fields, e.g., mechanical engineering, automotive engineering, robotics, and biomechanics. The formulation of the contact problems gives rise to variational inequalities, as the contact boundaries are part of the solution and are unknown apriori. Due to these reasons, it becomes essential to employ iterative solution methods to solve contact problems. At each iteration, the algorithm aims to satisfy equilibrium conditions for a given contact boundary. In many cases, the iterative schemes are computationally intensive and heavily rely on the geometric information of the problem. To address these challenges, we present a domain decomposition-based solution strategy for solving contact problems in a fully algebraic manner. In this work, we employ a dual Lagrange multiplier-based mortar Finite Element method for discretization. In addition, we also apply a Householder reflection to transform the local coordinate system such that the linear contact constraints can be transformed into point-wise constraints. Once the algebraic system is constructed, we must solve a sequential quadratic programming problem. To this aim, we employ a sub-structuring domain decomposition-based strategy that decomposes the domains in non-overlapping subdomains. Using these non-overlapping subdomains, we decouple the unknowns into the interior of the subdomains and the ones that are on the interfaces and the contact boundary. By employing this decomposition, we eliminate the interior unknowns and construct a smaller subproblem on the skeleton, which is subjected to inequality constraints. Once we have constructed a smaller constrained optimization problem, we can solve it using projection-based methods. This robust approach allows us to solve large-scale problems using a distributed computing environment.Finally, we will present some numerical results to demonstrate the performance of our method using several numerical examples. We will test our solution strategy for solving the contact problem with hyperelastic material with multiple bodies in two and three dimensions.

Machine learning algorithms for accelerating material characterization, discovery, design, and manufacturing processes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DISCOVERY OF CONDUCTIVE INKS AND ELECTRONIC DEVICES CO-DESIGNED WITH CLOSED-LOOP, AUTONOMOUS, REINFORCEMENT ECOSYSTEMS

Matthew Kottwitz[*1] and James Fowler*[1]

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ABSTRACT

The end-to-end design and manufacturing of printed circuit boards substrates, a ubiquitous and critical technology in energy storage, communication, and defense systems, is poised to undergo a transformation following developments in additive manufacturing within the last decade. These advancements include droplet-on-demand inkjet printing of conductive inks—suspensions of metallic nanoparticles, graphene, carbon nanotubes, etc.—onto dielectric substrates. Despite extensive research, few printed commercial inks possess the conductivity and robustness desired by high-reliability design agencies. A major contributor to the limited availability of viable inks is the enormous parameter space of processing conditions and material structure, property, and performance criteria that must be balanced during development. For this reason, Sandia National Laboratories, together with university partners, has engaged in the design and implementation of an autonomous materials discovery platform to efficiently (1) synthesize Cu, Ag, and Au nanoparticles, (2) formulate those nanoparticles into inks, and (3) print those inks to form devices. At each step of the process, characterization data of the structure, properties, and performance is provided to a machine learning algorithm. Initial approaches have utilized off-the-shelf machine learning methods while development of bespoke solutions such as multifidelity reinforcement learning and scientific machine learning continues to address the challenges of relatively sparse data sets, multimodality and fidelity, and the need identify underlying process-structure-property-performance relationships.

Physics-based data-driven modeling and uncertainty quantification in computational materials science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CAPTURING MODEL-FORM UNCERTAINTIES IN VARIOUS MOLECULAR DYNAMICS ENSEMBLES WITH STOCHASTIC REDUCED-ORDER MODELING

Senou Kounouho[1], Chongze Hu[2], Remi Dingreville[3] and Johann Guilleminot[1]*

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[2]*University of Alabama*
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ABSTRACT

This talk focuses on the representation of model-form uncertainties in various molecular dynamics ensembles. In prior contributions, the modeling of such uncertainties was formalized and applied to quantify the impact of, and the error generated by, pair-potential selection in the microcanonical ensemble (NVE). In this work, we extend this formulation and present a linear-subspace reduced-order model for the canonical (NVT) and isobaric (NPT) ensembles. We randomize the reduced-order basis on the tangent-space of the Stiefel manifold to provide topological relationships and capture model-form uncertainty. Using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS), we assess the relevance of these stochastic reduced-order atomistic models on problems for Lennard-Jones fluid and Cu-Al segregation energy simulations.

UQ-TTA student paper competition in uncertainty quantification
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CAPTURING MODEL-FORM UNCERTAINTIES IN VARIOUS MOLECULAR DYNAMICS ENSEMBLES WITH STOCHASTIC REDUCED-ORDER MODELING

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Recent advances in numerical methods for mixed-dimensional PDEs
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BACKWARD DIFFERENCE FORMULAE FOR THE TRANSIENT STOKES PROBLEM: OPTIMAL ORDER VELOCITY AND PRESSURE ESTIMATES

Alessandro Contri[1], *Balázs Kovács**[2] *and André Massing*[1]

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ABSTRACT

In this talk we will present a new stability and error analysis of fully discrete approximation schemes for the transient Stokes equation.
The numerical method uses backward difference formulae (BDF methods) of order 1 to 6 in time and a wide class of Galerkin finite element methods including both inf-sup stable spaces and symmetric pressure stabilized formulations.

We perform a unified error analysis for the above method, and prove stability of the method and show optimal-order error estimates for both the velocity and the pressure. The main tools in our stability analysis is the G-stability theory of Dahlquist together with the multiplier technique introduced by Nevanlinna and Odeh.
We will report on various numerical experiments.

The talk is based on joint work with Alessandro Contri and André Massing (NTNU Trondheim).

Advances in computational biomechanics and mechanobiology
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A FRAMEWORK FOR UNDERSTANDING VASCULAR REMODELING: FROM GEOMETRY TO TRANSPORT DYNAMICS.

Jérôme Kowalski[*1], Lorenzo Sala[2], Dirk Drasdo[1] and Irene Vignon-Clementel[1]*

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ABSTRACT

A number of diseases affect perfusion and function of organs. Liver cirrhosis is a complex and widespread disease. A better understanding of the consequences of its development on the organ would allow for more effective treatment. Cirrhosis affects the liver's vascular network as it remodels around the cirrhotic nodules. Quantifying the alterations of the vascular network permits to predict the resulting hemodynamic shifts and the modified transport of chemical substances entering the organ. Contrast-enhanced dynamic imaging offers a means to evaluate organ perfusion in diseased states. However, quantitatively interpreting dynamic imaging is a non-trivial task that requires modelling the transport of species within the vascular network. Current reduced models unfortunately lack information on the network geometrical characteristics. We here present a mechanistic model of an organ vascular network, aiming at unraveling how vascular remodeling affects the organ's hemodynamic and transport features.

Based upon the concept of structured binary trees [1], the model constructs vessels iteratively from a root vessel until the terminal vessels' radius reach a threshold. Fixed area ratio and power law index for the entire tree enable to deduce the two downstream vessel radii from an upstream vessel radius at each bifurcation. The length-to-radius ratio of each vessel is also fixed. Steady hemodynamics, computed by Poiseuille law, with an imposed pressure difference at the boundaries, are the basis for transport of the injected substance. The substance is injected in the root vessel and follows blood flow in each branching vessel via advective transport. The substance collected at terminal vessels is compared to the injected profile forming the transfer function which characterizes the linear transformation induced by the tree.

This framework allows to describe simulated transport behaviors through the architecture of the vascular network. Notably, as the asymmetry of a tree increases, the substance transport displays a behavior similar to that of diffusion – otherwise absent from the model. This behavior aligns best with a Gamma distribution of the exiting times and lies halfway between the two commonly used models for transport in an organ. Furthermore, as a vascular tree remodels during disease progression, the geometric parameters of the model evolve, mirroring the remodeling process. This study lays the groundwork for characterizing and comparing liver vascular structures throughout cirrhosis development, offering valuable insights into disease progression.

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Data-driven modeling and design of materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFICIENT COMPUTATIONAL HOMOGENIZATION OF MATERIALS WITH RANDOM MICROSTRUCTURE MORPHOLOGY THROUGH ENHANCED MACHINE LEARNING TECHNIQUES

Sergey Kozinov[*1], Niklas Miska[1] and Daniel Balzani[1]*

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ABSTRACT

The optimization of macroscopic material properties for specific engineering requirements by the utilization and adaption of heterogeneous microstructures gained increased interest in the last years. The challenge therein lies in accurately predicting the uncertain macroscopic behavior resulting from a variability in the microstructure's morphology. Building on the method proposed in [2], this contribution introduces an approach using machine learning to enhance the efficiency and by that, the design of artificial microstructures for computational homogenization.

In this study, we advance the concept of statistically similar representative volume elements (SSRVEs) [1] to create artificial microstructures that statistically replicate real microstructure morphologies. The original method, as detailed in [2], relied on extensive numerical simulations using the Finite Element Method (FEM) to homogenize microscopic mechanical fields, facing challenges in achieving accurate statistics for macroscopic material properties due to the associated numerical costs. Our approach overcomes these challenges by integrating machine learning into the process, which allows the evaluation of an increased number of microstructure samples.

The technique is demonstrated with an application to a dual-phase steel, characterized by a martensitic phase fraction within a ferrite matrix. Artificial microstructures with ellipsoidal inclusions are constructed, such that the morphology of the entire set varies similar to the real material. Based thereon, the machine learning model is constructed, such that the characterizing parameterization of the microstructure's morphology as input yields macroscopic material properties as output. This method shows remarkable efficiency improvements and is set to extend to more complex scenarios, such as a fully coupled FE2 calculation.

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Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREDICTING ELASTIC AND INELASTIC FRACTURE OF PERIODIC BEAM-BASED ARCHITECTED MATERIALS USING A MIXED-ORDER QUASICONTINUUM METHOD

Kevin Kraschewski[1] and Dennis Kochmann*[1]

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ABSTRACT

Predicting the failure mechanisms of low-density periodic architected materials has been a challenge for computational mechanics. One of the key differences between these materials and classical monolithic solids is their discrete nature of failure. Shaikeea et al. [1] found that even for brittle base materials that are linear elastic up to failure, this gives rise to significant differences in fracture behavior compared to continuous media.
Their fabricated specimen contained up to ten million, periodically arranged, unit cells (UCs), resulting in finite element (FE) simulations with up to a billion degrees of freedom. To investigate fracture in large manufacturable specimens, FE simulations are too costly, especially if the inelastic behavior of commonly used base materials in additive manufacturing is modeled.
Therefore, multiscale techniques become the method of choice. However, classical hierarchical homogenization techniques rely on the assumption of a separation of scales. When this assumption breaks down, e.g., in fracture mechanics, such techniques fail. Therefore, we present a concurrent multiscale technique, viz., a fully-nonlocal quasicontinuum (QC) multi-lattice formulation based on a conforming mesh. Our QC formulation is applied to trusses, whose struts are represented by a corotational beam model with cross sections discretized by fibers [2]. Each fiber's material response relies on an incremental variational description, allowing a thermodynamically consistent formulation. The overall setup captures significant nonlinearity and localization effects in fully-resolved regions, while efficiently approximating the remaining simulation domain through a coarse-graining technique. Coarse-graining is achieved by selecting representative UCs (RepUCs) and introducing geometric constraints based on interpolation, here exploiting finite-element interpolation.
Previous studies showed that within coarse-grained regions the strain energy of bending-dominated lattices undergoing non-uniform deformation is overpredicted when using affine interpolation. To overcome the overprediction, we introduce higher-order interpolation in coarse-grained regions, while using affine interpolation in the discrete, fully-resolved domain.
In conclusion, we present an efficient multiscale framework to investigate inelastic and linear elastic fracture of bending- and stretching-dominated periodic beam-based metamaterials. The method is equivalent to a fully-discrete calculation in certain regions, e.g., near the crack flank, where every UC is also a RepUC, but is significantly more efficient in coarse-grained regions.

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Boundary element methods: New theories and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE METHOD OF BOUNDARY INTEGRAL EQUATIONS IN THE BOUNDARY VALUE PROBLEMS OF DYNAMICS OF FLUIDS AND GASES

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ABSTRACT

The numerical experiment has become widely applicable alongside the physical one due to multiple parameters and the non-linearity of the main problems of continuum mechanics. Significant achievements are recognized in the computational analysis, especially in numerical implementation of particular mathematical models in mechanics [1]. In gas mechanics, significant progress has been achieved in viscid gas mechanics that takes into account physical and chemical processes, which allows determining aerodynamic characteristics in transonic flight modes and creating real-time computational models. Viscid gas dynamics pays the most attention to qualitative methods of formalization of initial boundary value problems, which lead to creation of the new mathematical models raising new questions and allowing solutions for the problems of viscid gas flows at low and medium Reynolds numbers. In the aerodynamics of complex lift-generating systems, the method of boundary-integral equations and variants of its numerical implementation was used to obtain the distributed and integral aerodynamic characteristics for two- and three-dimensional loadbearing forms and to study processes that cause flow separation, creation and stability of vortex structures.

The method of boundary integral equations has obvious and proven advantages over the finite difference and finite element methods. Reducing a boundary value or initial boundary value problem to an integral equation or an adequate system of boundary integral equations allows not only to reduce the dimension of the problem, but also, due to the analytical representations of solutions, to solve problems of optimization of aerohydrodynamic characteristics [2].

Generalization and development of the boundary integral equation method onto dynamic problems of interaction between viscid gas flow and a finite span wing of an arbitrary spatial form have been presented. Existence of a vector potential of the momentum conservation law is established for the first time. Further, analytical integral representations of the solutions of general conservative forms of differential conservation laws of fluid mechanics have been obtained.

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Data-driven device and circuits models
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PROJECTION-BASED REDUCED-ORDER MODELS FOR COMPACT CIRCUIT MODELS

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ABSTRACT

This work presents the use of projection-based reduced-order models (ROMs) using Proper Orthogonal Decomposition (POD) with Galerkin projection to reduce the computational expense of compact models within Spice simulations. The work focuses specifically on modeling compact models within Xyce, Sandia's circuit simulator code.

Galerkin POD is generally applied to systems of nonlinear partial differential equations (PDE) [1]. These PDEs have many degrees of freedom, e.g., a spatial domain, that allows for Galerkin POD to significantly reduce the size of the system being solved by reducing the system from a PDE to an ordinary differential equation. Spice compact models consist of systems of differential algebraic equations that do not necessarily have a large "spatial" domain. This presents a challenge for creating Galerkin POD ROMs for Spice compact models.

Model order reduction using Galerkin POD has been used for Spice models with varying degrees of success and challenges, usually projecting along the state space [2, 3]. A "spatial" component can be recovered by chaining subcircuits together, but this inherently limits the use of ROMs for Spice models. Similar to hyper reduction for ROMs applied to PDEs, techniques such as Missing Point Estimation are needed to see a significant reduction in computational expense for Galerkin ROMs of Spice models [2].

In this work, instead of projecting along a state space or "spatial" domain, we project the residual equation of the compact model along a parameter domain. This approach, which is admittedly case-dependent, was able to (1) generalize the method for any subcircuit, (2) reduce the size of the system of DAEs of the compact model, and (3) predict accurate solutions across different parameter points in the domain.

Results for the projection-based ROMs for the compact models will be presented for three circuits: a nonlinear capacitor circuit, a nonlinear capacitor and diode circuit, and a nonlinear transmission line. Results are shown for how well the projection-based ROMs can predict solutions in the parameter domain and how much computational speedup the ROM achieves compared to the full-order model.

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IMMERSED DOMAIN APPROACH FOR FLUID-STRUCTURE-CONTACT INTERACTION PROBLEMS

Maria Giuseppina Chiara Nestola[1], Patrick Zulian[12], Hardik Kothari[1] and Rolf Krause[*12]*

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ABSTRACT

We present an embedded approach for the numerical solution of contact problems be- tween multiple elastic structures immersed in a fluid flow. Our parallel approach is designed to simulate the full dynamics of a bio-prosthetic heart valve. We model the blood-valve interaction, the blood-aortic wall interaction, and the contact among leaflets during the valve closure. The solid bodies are modeled as hyperelastic and anisotropic materials, whereas the fluid is regarded as a Newtonian flow. The mathematical modeling of such material properties and the contact mechanics give rise to a large-scale nonlinear problem that is both challenging and computationally expensive to solve. We employ a localized version of the L^2-projection for handling the fluid-structure vol- umetric coupling and a variant of the mortar method for coupling the surfaces of the structures in contact.
In this contribution, we describe our approach to solving the contact problem between the immersed solids. First, we provide an algorithmic overview of the FSI algorithm, which is specifically designed to include and fully resolve the contact constraints. Second, we illustrate our parallel large-scale solution strategies for solving the arising contact sub-problem in a non-smooth optimization framework. The proposed strategy is validated and finally employed to model the dynamics of a bio-prosthetic heart valve placed in the aortic root.

Smart structures – Modelling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

OPTIMIZED FORCE MANIPULATION IN ADAPTIVE TRUSS STRUCTURES USING INSIGHTS FROM STRUCTURAL MECHANICS

Lisa-Marie Krauß[1], Mathias Maierhofer[1], Achim Menges[1] and Manfred Bischoff[1]*

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ABSTRACT

Growing worldwide issues like resource scarcity and climate change are in large part caused by the construction sector. Therefore, rapid development of promising solutions is necessary to speed up the transformation of the construction sector. One potential strategy to tackle this challenge is investigated by the University of Stuttgart's collaborative research center CRC 1244 “Adaptive skins and structures for the built environment of tomorrow”. Control units, actuators and sensors are integrated into civil engineering structures to enable them to adapt flexibly to varying load scenarios. This can extend the service life of buildings and save a significant amount of material [1].

In the CRC a variety of topics, including design, dimensioning and operation of adaptive structures, is examined. Design studies have demonstrated that stiffness-governed structures can be transformed into strength-governed structures through the use of actuators, resulting in a significant reduction in the amount of material required [2]. Furthermore, actuators allow to manipulate the forces in the structure during operation. One possible aim is to minimize the maximum utilization ratio in the structure to avoid too high utilization ratios in individual elements. To achieve this, the actuator strokes are adjusted in response to the loads.

In this contribution, we present our approach to treat this task as an optimization problem, where the highest cross-sectional utilization ratio in a truss structure is minimized and the actuator strokes serve as design variables. We formulate the optimization problem mathematically and apply insights from structural mechanics to simplify it. The objective function is identified as a convex function. Instead of searching on the initial objective function, which is convex but non-differentiable, a further reformulation allows searching in the convex set. As a result, the linear optimization problem can be conveniently solved using the simplex method. Finally, we illustrate opportunities and limitations of force manipulation in adaptive structures using various examples.

The work described in this contribution was conducted within the Collaborative Research Center 1244 “Adaptive skins and structures for the built environment of tomorrow”, funded by the Deutsche Forschungsgemeinschaft (German Research Foundation) under project number 279064222. This support is gratefully acknowledged.

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Scientific deep learning
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A SENSITIVITY APPROACH FOR DEEP NEURAL ARCHITECTURE ADAPTATION

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ABSTRACT

This work presents a novel algorithm for progressively adapting neural network architecture along the depth. In particular, we attempt to address the following questions in a mathematically principled way: i) Where to add new capacity (layer) during the training process? ii) How to initialize the new capacity? The algorithm is based on defining the sensitivity for a neural network which is conceptually the derivative of a lost function with respect to infinitesimal changes in the neural network. Using an optimal control viewpoint, we show that the network derivative exists under certain conditions and a closed-form expression for the same is derived. Further, we show that the derived expression for the topological derivative leads to an eigenvalue problem for deep neural architecture adaptation. The algorithm we derived simply determines the most sensitive location along the depth where a new layer needs to be inserted during the training process and the associated parametric initialization for the newly added layer. We also show that our layer insertion strategy based on the topological derivative approach can be viewed as a solution to a constrained optimization problem in the infinity-Wasserstein space. Numerical investigations with feed-forward networks (fully connected network and convolutional neural network) on prototype regression and classification problems demonstrate that our proposed approach can outperform an ad-hoc baseline network and other neural architecture adaptation strategies.

Design and mechanics of mutifunctional composites and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RITTER-KRIŽAIĆ ITERACION METHOD OF TRUSS CONSTRUCTIONS

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ABSTRACT

The optimization of the dimensioning of constructive designs is constantly evolving. FEM, evolutionary, and other various methods are being developed, which are implemented with algorithms in computer simulations of building models. The problem with these methods is solving large differential equations, which is inconceivable without computers and large memories. The Ritter-Križaić (RK) iteration method works for both straight and oblique networks with one side, and it can even be used instead of trigonometric and FEM equations. It does this by adding the geometric properties of the networks and outside actions to the directional equations. By creating straightforward monograms of RK-FEM technology (Fig.1) with straightforward differential or subspace equations that are simple to calculate by hand or draw with Mathcad tools, the RK-FEM loop enables COD to define various types of trusses and even other supports. RK-FEM COD is therefore used to create simulation games that explain many logical phenomena in the design of external and internal actions of beam supports, which can be compared to a spider thread or an ice plate structure as an RK string and even to the moon.

Computational mechanics in high-strain rate and impact engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPERIMENTAL AND NUMERICAL ANALYSIS OF BUCKLING OF THIN POLYETHYLENE STRUCTURE DURING DYNAMIC IMPACT LOADING

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ABSTRACT

Polyethylene is a semi-crystalline polymer that is widely used in the industry in general and in the packaging industry in particular. Dynamic, inelastic buckling of a polyethylene structure in the form of a package top is the focus of the present study.

A constitutive framework for the isotropic elasticity and inelasticity of HDPE is proposed. All state variables in the model are defined in the current state of the material, and the evolution of elastic deformations is prescribed directly. The proposed model was calibrated by use of uniaxial tensile tests. The uniaxial tests were carried out at different loading rates. Drop-testing was also performed by dropping a weight on the 3D geometry, which would then buckle. Also, a 3D numerical implementation of the constitutive model was provided (VUMAT in Abaqus), and by use of this 3D implementation, the drop-testing could be simulated.

The results show that the air trapped inside the structure/top during the droptest needs to be included in the simulation model when simulating the droptests. In order to do this, a coupled Eulerian-Lagrangian (CEL) analysis, which is a kind of fluid-structure-interaction analysis, was employed. Through this type of analysis, the correct buckling scenario could be predicted in the numerical analysis. The droptests were recorded using a high-speed camera. The position and velocity profiles from the tests could then be compared to the simulations. In general, the simulations showed very nice agreement with the experimental measurements.

Advanced analysis of steel and steel-concrete composite structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOWARDS COMPOSITE BEAM ELEMENTS FOR STEEL TRUSS IN CONCRETE COMPOSITE BEAMS

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ABSTRACT

Steel composite construction is a discipline in civil engineering that strives for efficient structural members through a reasonable combination of a steel section with another material. The most popular steel composite structures are certainly steel-concrete composite beams consisting of a concrete slab on a downstand steel profile connected through shear studs. After decades of research, this type of structure has become a popular solution in the construction industry, especially for multi-storey buildings with large spans. Accurate and reliable structural analysis of such composite sections requires careful consideration of the material non-linearities as well as the deformability of the shear connectors coupling both components. Newmark et al. [1] approached this subject both experimentally and analytically by proposing a first kinematical model of the interlayer slip between the components. This model has been pioneering for the development and successful implementation of composite beam elements in the framework of finite element methods. In recent times, technical developments in steel-concrete composite construction have focused more on shallow steel-concrete composite beams consisting of a steel profile partially embedded in concrete. The European Norms for composite construction (EN 1994-1-1) do not exclude slim-floor beams from their scope but a more comprehensive design approach is recommended. For example, the design checks for the shear connection shall be based on experimental tests and a conceptual model unless headed stud shear connectors are used. Whilst this suggestion accounts for the resistance of the shear connection, the computation of the shear connector load effects remains pivotal. More precisely, the accurate determination of the shear connectors' forces and deformations is not straightforward in the ultimate limit state due to the material non-linearities of the components and their interaction. Composite beam elements are commonly still unavailable for shallow steel-concrete composite beams while being potentially suitable to fill this gap. The proposed contribution thus presents a numerical framework for shallow composite steel truss and concrete (CSTC) beams that was inspired by companion numerical investigations on conventional composite beams. It intends to emphasize first the role of the kinematics in the development of composite beam elements and to present the full-scale beam tests conducted with the specific type of slim-floor beams under investigation to study the kinematics and finally validate the numerical framework developed.

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Design beyond optimization: Why, what if, and how much?
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GRADIENT-BASED LAYOUT OPTIMIZATION FOR EFFICIENT 3D PACKING OF COMPLEX COMPONENTS

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ABSTRACT

There is an ever-growing need for effective integration of advanced technologies into limited spaces. This challenge is relevant across diverse industries such as aerospace, automotive, and electronics, where optimizing the layout of components within a system can enhance overall system performance, reduce cost, and maximize space utilization. Component layout optimization is a complex non-linear multimodal problem that poses substantial challenges for traditional optimization methods. To manage these complexities, design spaces are often discretized into predetermines potential component locations, leading to a significant limitation in design freedom. Moreover, many existing tools in this domain tend to focus narrowly on placing components based on a small number of application-specific parameters, such as heat transfer or mass distribution. These approaches often overlook other simpler, but critical aspects necessary for a feasible and realistic design. A layout that is mathematically optimal but overlooks even one basic requirement, such as mounting or accessibility, becomes unfeasible for practical application. In real-world scenarios, the complexity of these problems is amplified when considering multiple engineering parameters. Developing a layout that not only meets all essential requirements for feasibility and practicality but also considers more specialized, application-specific parameters, all while ensuring complete design freedom for the parts, is not merely desirable but imperative for future layout optimization tools.

This work outlines a novel gradient-based layout optimization method tailored for 3D packing of complex geometries. This approach provides full translational and rotational freedom for all components while considering parameters such as packing space, part overlap, mounting requirements, proximity relationships, accessibility constraints, and connection distances. To demonstrate the effectiveness of this approach, both academic and industry-related test cases were used. In one such industry application, the method achieved a notable 68% increase in packing density when focusing solely on packing space. When the problem statement was updated to include both mounting and cable length considerations, a 14% increase in packing density was achieved, coupled with a 19% reduction in cable length, underscoring the versatility and efficacy of the optimization method. This research holds promise for substantial advancements in the field of component layout optimization, offering practical benefits in both academic and industrial settings.

Computational mechanobiology of musculoskeletal tissues
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INTEGRATING OSTEOBLAST MECHANICS AND BEHAVIOURS IN A DISCRETE CELL-BASED MATHEMATICAL MODEL FOR BONE TISSUE FORMATION

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ABSTRACT

During bone tissue growth, active bone-forming cells (osteoblasts) proliferate and embed into the extra-cellular matrix that they produce to form new bone tissue. This growth occurs in confined spaces with complex geometries, such as resorption cavities in cortical bone and trabecular resorption pits. Restricted available space in these geometries causes the progression rate of the new bone tissue interface and the density of osteoblasts to be highly regulated by local geometry, resulting in what is called geometric control of tissue growth [1]. While the effects of geometry during tissue growth are established, empirical observations also suggest cellular mechanics significantly influences the growth process [2,3]. Furthermore, particularly around cylindrical cavities such as Haversian canals in cortical bone, the deposition rate of new tissue material slows down as the growth process progresses. This slowdown can be attributed to the decrease in the population of active osteoblasts due to cell death and the embedment of osteoblasts as osteocytes into new bone tissue.

In this contribution, we present a discrete, cell-based mathematical model of osteoblast forming new bone tissue to explore how the rate and pattern of bone tissue growth depends on osteoblast cell-cell mechanical interactions and the stochastic embedment of osteoblasts as osteocytes into newly formed bone tissue. Our model effectively replicates two key phenomena seen experimentally: the smoothing of the initial geometry of resorption cavities, and the slowdown of new tissue deposition. Additionally, our discrete model provides the positions of osteocytes generated during bone formation, enabling further research into their distribution.

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A DISCONTINUOUS GALERKIN FINITE ELEMENT MODELING APPROACH FOR COMPOUND FLOODING EVENTS

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ABSTRACT

Storm surge finite element models are essential tools in helping to assess the extent and severity of coastal flooding associated with tropical cyclones (TCs); however, the flooding that occurs during these storms is often generated by both surge and accompanying rainfall, resulting in a so-called compound flooding event, which U.S. cities are under increasing risk of experiencing [1]. Simulating compound flooding events requires a modeling framework that extends beyond the "standard" capabilities of storm surge models, which generally account for surges in water levels driven by TC winds and pressures, but not by the accompanying (often torrential) TC rainfall. To address this shortcoming, we develop a local discontinuous Galerkin (LDG) finite element method for modified shallow water equations, which include, in addition to momentum source terms due to TC winds and pressures, a mass source term in the continuity equation to represent TC rainfall [2]. Central to our modeling approach for these terms is the estimation of the TC winds, pressures, and rainfall by use of parametric storm models, which exploit the defined structures exhibited in TC meteorological patterns. This approach allows us to construct the TC meteorological fields using (relatively) simple analytic expressions that are a function of a small number of (predicted or observed) storm parameters (e.g., the storm center, maximum sustained wind, etc.) — parameters that are made publicly available by various weather agencies, such as the National Hurricane Center (NHC), both pre and post storm events. The developed modeling framework is used to simulate compound flooding due to both storm surge and rainfall for a number of TCs making landfall in the US, where our results demonstrate that improved peak water levels are obtained compared to modeling surge alone and highlight the potential of using parametric TC rainfall models in compound flood simulations.

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Mathematics and algorithms for predictive digital twins (DT)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PARTITIONED COUPLING OF MULTIFIDELITY, MULTIPHYSICS MODELS USING OPTIMIZATION-BASED COUPLING

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ABSTRACT

Problems involving coupling over a nonoverlapping interface abound, with common examples including virtual interfaces introduced for the purpose of domain decomposition and physical interfaces such as are found in, e.g., multimaterial solid interaction and fluid-structure interaction. Although monolithic formulations for such problems can be developed, they can be very challenging to solve once posed, due to the large size of the resulting nonlinear systems of algebraic equations. Partitioned approaches for solution of coupled problems enable the use of subdomain solvers developed by domain experts and are more amenable to a “plug-and-play” style of framework. However, with partitioned approaches, considerable attention must be given to enforcing coupling conditions.

As model reduction techniques continue to mature, it is natural that there is a desire among analysts to use cheaper, more efficient models where possible. This fits closely with the partitioned approach to solving coupled problems. It is towards this goal of solving multifidelity coupled problems involving reduced order models (ROMs) and full order models (FOMs) that we extend a partial differential equation (PDE) constrained optimization technique, developed for elliptic FOMs [1] and later extended to parabolic FOMs [2] and multiphysics [3], to ROM-ROM coupling.

The use of a ROM in one or more subdomains allows for harnessing their efficiency, but also presents a challenge with respect to reduced adjoint systems required to be solved as part of the technique. We explore the ROM-ROM coupling technique, applying it to coupled advection-diffusion equations. We present numerical studies demonstrating the accuracy of the approach along with an investigation related to selecting a reduced order basis for the adjoint systems.

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Emerging frontiers and methods in digital manufacturing: Modeling, simulation, and beyond
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING THE DIRECT INK WRITE PROCESS USING A SHARP INTERFACE FINITE-ELEMENT METHOD

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ABSTRACT

Direct Ink Write (DIW) is an additive manufacturing technique that allows for the creation of complex patterns by extruding an “ink” material through a syringe onto a substrate; it is used in a variety of applications from biological systems to electronics. The printing process requires inks with complicated rheological properties, including shear thinning to be extrudable and yield stress in order to hold their shape. Modeling DIW presents many challenges for computational models, which include the highly nonlinear behavior of materials, as well as tracking of the complex material interfaces as the ink is deposited onto the substrate. We simulate the DIW process using finite-elements to solve the transient, three-dimensional Navier-Stokes equation using a non-Newtonian viscosity model to capture the effects of the complex ink rheology. To track the ink/air/substrate interfaces a sharp interface method is used, known as the conformal decomposition finite-element method (CDFEM). CDFEM is a conformal meshing algorithm that creates sharp boundaries between materials, which allows for the application of boundary conditions such as capillarity and to accurately capture discontinuities in properties such as density or viscosity between materials. In this talk, we will present the results of our simulations of the DIW process. In particular, we will investigate the ability of our computational model to predict a DIW printing failure mode when there is a mismatch between the substrate velocity and extrudate deposition rate. For a given extrudate deposition rate, a relatively fast-moving substrate can cause defects in the printed pattern, allowing discontinuities in the printed pattern where none should be present. We will compare our modeled results to our existing experimental data for both Newtonian and non-Newtonian inks.

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PARAMETER AND DOMAIN-ROBUST PRECONDITIONERS FOR COUPLED MULTIPHYSICS PROBLEMS

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ABSTRACT

Mathematical modeling of the so-called glymphatic system at the macroscale is based on multiphysics systems describing the interaction of the porous media flow and the viscous free flow. Here, interaction of the two subsystems, wide ranges of parameter regimes and importantly also the problem geometry (notably the domain's aspect ratio) present a difficulty for establishing robust and efficient solution algorithms. Focusing on the coupled Stokes-Darcy system [Layton 2002, Discacciati 2002] as a model problem we discuss in this talk monolithic and domain decomposition preconditioners which address these challenges.

Advances in multi-scale, multi-material, and multi-component Topology Optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STRESS-BASED TOPOLOGY OPTIMIZATION FOR ROLLER-BOX DESIGN IN ADDITIVE MANUFACTURING, INCLUDING BUILD PREPARATION

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[1]Cenaero

ABSTRACT

The design freedom and local control over material properties provided by additive manufacturing are key advantages compared to traditional methods. Fully harnessing these benefits poses a complex challenge that questions intuitive design approaches. In response to these challenges, we developed Morfeo, an in-house software solution specifically tailored to address the complexities of AM design. Two topology optimization strategies are available in MORFEO and combined : the density method (SIMP) which parameters the design by material densities, and an XFEM Level Set method with an explicit (extended finite element) representation of the void-solid interfaces. We show here the integration of specific aspects of additive manufacturing into the design process.

Expanding our capabilities, a novel staged optimization loop, powered by the advanced in-house tool Cafeine, enhances additive manufacturing preparation. Swiftly analyzing critical manufacturing areas, it surpasses mere analysis by detecting closed cavities, evaluating roughness, sensing recoater impacts, identifying support needs, estimating volume, assessing depowdering risks, pinpointing cross-section changes, and evaluating manufacturing time. Integrating part preparation early in the design stages, we aim for a more integrated, efficient design process tailored to manufacturing requirements, fostering design innovation.

The effectiveness of the approach is vividly demonstrated in the redesign of a roller box, where a remarkable 30% reduction in mass was achieved compared to the existing concept, while still fulfilling the stress-based criterion. Moreover, this optimization strategy seamlessly integrates into our part design processes, underscoring its positive impact on both structural performance and the manufacturability of AM components.

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Advanced materials and smart structures: Modeling, simulation and testing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SELF-HEALING CONCRETE COMPOSITES: MODELING AND EXPERIMENTS

Mieczyslaw Kuczma[*1], Alireza Tabrizikahou[1], Marcin Wysokowski[1], Isaac Agbamu[1], Magdalena Lasecka-Plura[1], Jan Bialasik[1] and Peter Wriggers[2]*

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ABSTRACT

Concrete is the most widely used construction material due to its high compressive strength, local availability of raw materials and simple production methods. However, it is a brittle material with low tensile strength resulting in occurrence of micro-cracks, which reduce the durability and stiffness of the concrete structure and may successively lead to a loss of its structural integrity.

This presentation introduces a novel approach to address concrete crack-closure utilizing capsules laden with a biogenic healing agent alongside shape memory alloy fibers. Drawing inspiration from biomineralization processes, a cutting-edge method for the fabrication of these capsules will be unveiled and thoroughly examined using various modern analytical tools like AFM, SEM, FTIR, TG. This pioneering methodology not only holds promise for enhancing the durability and performance of concrete structures but also underscores the transformative potential of biomineralization-inspired strategies in materials science and engineering. Through elucidating the synthesis and application of these innovative capsules and healing agents, this presentation endeavors to propel the advancement of sustainable, resilient construction materials into the future.

The results of in-house laboratory experiments on such concrete composites as well as the modeling and simulation of the deformation and healing processes will be presented and discussed, using the concepts of thermodynamics and phase-field approach and finite element approximation [1, 2].

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SciML in the real world
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AUTOMATED MODEL DISCOVERY FOR SOFT MATTER SYSTEMS

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ABSTRACT

Sparse regression and feature extraction are the cornerstones of knowledge discovery from massive data. Their goal is to discover interpretable and predictive models that provide simple relationships among scientific variables. Statistical tools for model discovery are well established in the context of linear regression; yet, in solid mechanics, model discovery typically translates in a nonlinear regression problem that remains incompletely understood. Here we explore model discovery and sparse regression through the lens of Lp regularization using data from the human brain [1], arteries [2], and artificial meat. Lp regularization introduces two hyperparameters: the power p by which it penalizes individual terms, and a penalty parameter by which it scales the relative importance of regularization and regression [3]. Our study reveals that L0 regularization is the only member of the Lp family that explicitly allows us to fine-tune the balance between interpretability and predictability, simplicity and accuracy, and bias and variance. We demonstrate that its penalty parameter acts as a discrete switch to select the desired number of terms. While L0 regularization across all possible models translates into an expensive NP hard discrete combinatorial problem with 2^n possibilities, our results suggest that beginning any discovery by performing L0 regularization for all possible one- and two-term models provides quick and valuable insight into the nature and hierarchy of the best-in-class models. Taken together, our study reveals the importance of L0 regularization in model discovery, because it is honest, transparent, and unbiased. We anticipate that our results will generalize to alternative discovery techniques including neural networks and symbolic regression, and to other domains including biology, chemistry, or medicine. Our ability to automatically discover material models from data could have tremendous applications in generative material design and open new opportunities to manipulate matter, alter properties of existing materials, and discover new materials with user-defined properties.

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Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MESHFREE: MINIMAL EFFORT FOR BEST QUALITY. ENSURE RELIABILITY OF INDUSTRIAL SIMULATION APPLICATIONS IN FLUID AND CONTINUUM MECHANICS.

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ABSTRACT

MESHFREE (meshfree.eu) is a simulation tool that originates from Fraunhofer ITWM (Germany) and is currently developed in cooperation with Fraunhofer SCAI. It is designed to solve industrial and scientific problems in fluid and continuum mechanics. Its geometrical basis is a non-meshed point cloud which moves (in Lagrangian sense) with the velocity of the continuum. The basis of approximation is a specific moving-least-squares-approach (MLS) together with a dedicated quality optimization. Both together provide a desired order of approximation accuracy as well as numerical stability.

Due to its design, MESHFREE is especially capable to address problems with dynamic free surfaces and phase boundaries, complex geometries and kinematics, fluid-structure interaction, and complex physics such as expanding flows (evaporation/foaming) or freezing.

In order to proof quality/validity of MESHFREE simulation results, the classical way is to proof numerical convergence of the result upon refinement of the geometrical basis (using finer and finer resolution of the point cloud) and/or upon using higher orders of approximation. However, this way of quality-testimonial is often ignored in practical or industrial applications as it is both time and resource consuming. This, indeed, is a conflict.

MESHFREE can provide a practicable solution/relaxation to this conflict. On one hand, MLS allows to precisely estimate the local approximation errors and thus establish reliable quality measures of the simulation result. On the other hand, it is almost trivial to locally refine or coarsen the point cloud based on given quality targets.

In this way, MESHFREE can provide simulation results with user-requested quality. Moreover, if computational or time resources are limited, MESHFREE can provide the qualitatively best solution within the given resource-spectrum. This widely enhances the scope of industrial applicability of simulations of this method in general.

Based on two industrial examples (modelling of water wading in vehicle design, modeling of PUR-foaming processes in chemical engineering), quality-triggered adaptivity of MESHFREE simulations will be demonstrated. The numerical convergence of the method will be shown based on significant result parameters.

Current trends in phase-field modeling and computations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE REVISITED PHASE-FIELD APPROACH TO BRITTLE FRACTURE: APPLICATION TO THE DIAMETRAL COMPRESSION AND WING-CRACK PROBLEMS

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ABSTRACT

In a recent contribution, Kumar et al. (2020, 2022) have introduced a comprehensive macroscopic phase-field theory for the nucleation and propagation of fracture in linear elastic brittle materials under arbitrary quasistatic loading conditions. The theory can be viewed as a natural generalization of the phase-field approximation of the variational theory of brittle fracture of Francfort and Marigo (1998) to account for the material strength at large. This is accomplished by the addition of an external driving force—which physically represents the macroscopic manifestation of the presence of inherent microscopic defects in the material—in the equation governing the evolution of the phase field. Through comparisons with experiments in materials soft and hard under various loading conditions, it has been shown that this theory may be a complete phase-field theory of fracture for brittle materials.

This talk will focus on the application of the theory to two problems involving fracture under large compressive forces: (1) Brazilian fracture (diametral compression) test and (2) Wing-crack evolution test. Such problems have proved to be challenging for the classical phase-field models, and various energy splits have been proposed in the literature to accurately describe experimental observations. We will show that the theory of Kumar et al. can intrinsically capture the compression-tension asymmetry without requiring an energy split. Computational implementation of the theory will be discussed.

From an application point of view, this talk will discuss how the theory can be used to correctly interpret the results of the Brazilian fracture test to measure tensile strength. Our analysis shows that the formulas proposed by the latest ASTM standard for the Brazilian test generally do not yield correct values for the material's tensile strength. A new protocol is proposed to deduce the tensile strength of a material from a Brazilian test. Moreover, for the wing-crack evolution test, the analysis shows that wing cracks can be obtained even when the mode II fracture toughness is equal to the mode I fracture toughness, in contrast to previous claims in the literature that mode II fracture toughness has to be much higher.

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Emerging topology and shape optimization techniques in computational design of materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

OPTIMIZED LATTICE DESIGN FOR TAILORED FORCE-DISPLACEMENT CHARACTERISTICS

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ABSTRACT

Optimized frames are employed in various large deformation applications such as energy-absorbing lattices, load-carrying structures, and compliant mechanisms. This study focuses on the development of an optimized lattice design leveraging advanced techniques for differentiation (auto-diff) and employing the Euler-Bernoulli beam theory. The objective is to tailor the force-displacement curve of energy-absorbing lattices to meet specific application requirements.

The computational framework utilizes auto-diff to efficiently compute derivatives for gradient-based optimization, allowing for the systematic exploration of design spaces. The Updated Lagrange method with Euler-Bernoulli beam theory is employed to model the non-linear mechanical behavior of the lattice structures using frame structures, providing a solid foundation for the optimization process. This integration of auto-diff and analytical modeling enables the generation of 3D lattice designs with enhanced performance in terms of force absorption and load-carrying capacity.

To validate the optimized lattice designs, a series of experiments are conducted to compare the predicted force-displacement curves with real-world physical behavior. Experimental setups involve the fabrication of prototypes using advanced manufacturing techniques such as 3D printing. The physical tests aim to confirm the accuracy and reliability of the computational models, ensuring that the optimized lattice structures perform as intended in practical applications.

The results demonstrate the effectiveness of the proposed approach in achieving the desired force-displacement characteristics in lattice structures. The experimental validation further strengthens the reliability of the computational predictions, providing confidence in the practical applicability of the optimized lattice structures in energy-absorbing and load-carrying applications. This interdisciplinary approach contributes to advancing the state-of-the-art in structural design with optimization, offering a powerful combination of computational efficiency and experimental validation for optimized lattice structures in large deformation scenarios

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Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTATIONAL OPTIMIZATION OF HIGHER-ORDER HOMOGENIZATION FRAMEWORK FOR LARGE-SCALE RVE MODELS

Athira Anil Kumar[1], Aewis K.W. Hii[1], Bassam El Said[1] and Stephen Hallett[1]*

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ABSTRACT

This study delves into the intricate computational challenges inherent in multi-scale modeling, particularly in the context of composite materials. The complexity arises from both generic and specific computational hurdles, such as the resolution of large system matrices and the management of dense constraint equations typical in higher-order homogenization frameworks. These issues are highlighted through the application of a second-order homogenization using thick shell elements proposed by Hii and El Said[1], with a focus on large-scale, finely-discretized Representative Volume Element (RVE) models. Such models are crucial for multi-scale modeling of complex structures like sandwich panels, porous and woven composites, where RVE sizes can become comparable to macro-scale models. Two primary computational challenges are highlighted through the downscaling and upscaling procedures of the framework. The downscaling procedure confronts the dilemma of handling large constraint equations in commercial finite element software, which typically have memory limitations on the size of elements or equations they can process. Conversely, the upscaling procedure underlines the task of solving large dense matrices to derive homogenized properties, such as ABD matrices. These challenges pose significant barriers to effective modeling and analysis, particularly in complex structures requiring fine discretization and high memory.
To address these challenges, our research proposes innovative solutions. For the downscaling procedure, Broyden’s method is employed iteratively to evaluate constraint forces. This method bypasses the conventional application of displacement boundary conditions to satisfy constraint equations. The iterative nature of this solution adapts seamlessly to complex non-linear problems while optimizing memory usage. Furthermore, this method has been extended to support multi-threaded parallelization, thus leveraging additional computational resources. Conversely, for the upscaling procedure, we leverage the use of Dask libraries, known for their effectiveness in handling extensive matrix systems via chunking. An adaptive approach is employed here, utilizing a conditional algorithm to select between static condensation or forward difference methods for the computation of ABD matrices, depending on specific model and computational conditions.
This new framework has been tested in various models requiring fine discretization and substantial memory resources. These include RVEs with embedded defects, sandwich panels, and 3D woven composites. The results demonstrate the framework's capability in effectively addressing and resolving the computational intricacies inherent in multi-scale modeling of complex structures.

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Phase-field models of fracture
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTATIONAL MODELING OF RATE DEPENDENT FRACTURE RESPONSE IN SOFT ELASTOMERIC MATERIALS

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ABSTRACT

Soft materials, owing to their low elastic moduli that are usually only a few KPa, can undergo extremely large deformations of up to several hundred percent strain prior to fracture. Such materials consequently present themselves as ideal constituent materials for a wide range of emerging cutting-edge biomedical applications such as tissue engineering and soft robotics [1]. This work deals with computational modeling of soft elastomeric materials exhibiting rate-dependent constitutive response, both in the pre-fracture as well as the fracture regimes, as revealed by an array of in-house experimental investigations conducted on representative materials of this class. A nonlinear finite viscoelasticity model based on the generalized Maxwell model is employed to capture the viscoelastic constitutive response. Further, we extend the finite-deformation elastic phase-field fracture model of [2] by introducing the dependence of fracture properties on the applied loading rate in order to capture the rate-dependent fracture response. The developed formulation is validated against experimental observations thereby providing useful insights regarding the rate-dependent fracture response of soft elastomeric materials.

Keywords: soft elastomers, viscoelasticity, phase-field fracture, constitutive modeling, experimental validation

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Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING RIBBONS/STRIPS AS A COSSERAT ROD

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ABSTRACT

This study presents a computational approach to obtain nonlinearly elastic constitutive relations of strip/ribbon-like structures modeled as a special Cosserat rod. Starting with the description of strips as a general Cosserat plate, the strip is first subjected to a strain field which is uniform along its length. The Helical Cauchy-Born rule is used to impose this uniform strain field which deforms the strip into a six-parameter family of helical configurations-the six parameters here correspond to the six strain measures of rod theory. Two vector variables are introduced to model the position of the deformed centerline of the strip's cross-section and to model orientation of thickness lines along the strip's width. The minimization of the strip's plate energy together with the aforementioned uniformity in strain field reduces the partial differential equations of plate theory from the entire mid-plane of the strip to just a system of nonlinear ordinary differential equations along the strip's width line for the above mentioned two vector variables. A nonlinear finite element formulation is further presented to solve the above mentioned set of ordinary differential equations. This, in turn, yields the strip's stored energy per unit length as well as the induced internal force, moment and stiffnesses of the strip for every prescribed set of six strain measures of rod theory. The proposed scheme is used to study uniform bending, twisting and shearing of a strip. For the case of uniform twisting and shearing, the strip is also seen to buckle along its width into a more complex configuration which are accurately captured by the presented scheme. We demonstrate that the presented scheme is more general and accurate than the existing schemes available in the literature.

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Advancements in model reduction, data assimilation, and uncertainty quantification for complex physical systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INVERSE UNCERTAINTY QUANTIFICATION OF INPUT FIELDS BASED ON IMAGE DATA WITH APPLICATION TO A TURBULENT SUPERCRITICAL CARBON DIOXIDE MIXING LAYER EXPERIMENT

Keishi Kumashiro[*1], Dhruv Purushotham[2], Joseph Oefelein[2], Adam Steinberg[2] and Masayuki Yano[1]*

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ABSTRACT

We present an inverse uncertainty quantification (UQ) framework for the input fields of complex fluid flows based on measurements that take the form of images. In particular, we demonstrate our framework on a turbulent supercritical carbon dioxide (sCO_2) mixing layer configuration that models an experiment designed and performed by researchers at the Georgia Institute of Technology (Lim C.H. et al. (2022) Proceedings of the ASME, Lim C.H. (2022) PhD thesis). Because of its proximity to the critical point of CO_2, the behaviour of the supercritical flow is sensitive to thermodynamic properties, namely pressure and temperature. In addition, while extensive measures have been taken to control the conditions on the boundary of the interrogation region, practical limitations inevitably introduce uncertainties in pressure and especially temperature boundary fields. As such, these fields must be accurately estimated to provide reliable predictions, and in our demonstration, we focus on estimating the temperature field at the inlet of the channel confining the mixing layer. Our approach to estimate and quantify the uncertainty of the inlet temperature field builds on the following four foundations. First, we model (i) the fluid dynamics using a large eddy simulation (Purushotham D. et al. (2022) AIAA SciTech Forum) and (ii) the planar laser Raman scattering measurements yielded by the experiment using an assortment of image synthesis methods of varying fidelity. Second, we approximate the inlet temperature in terms of a truncated Karhunen–Loève (KL) expansion, which recasts the field inversion problem into a parametric one. Third, we construct a rapidly evaluable likelihood function using (i) proper orthogonal decomposition of prescribed sets of synthesized, time-uncorrelated images and (ii) a surrogate model based on a cut high-dimensional model representation. Lastly, we approximate the posterior distributions of the KL coefficients using a Hamiltonian Monte Carlo sampling algorithm. We assess our framework using simulation-based solutions and synthesized images of the sCO_2 flow.

Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREDICTION OF PULSATING TURBULENT PIPE FLOW WITH EXTENSIVE DRAG REDUCTION EFFECTS BY DEEP LEARNING WITH GENERALIZATION CAPABILITY

Sota Kumazawa[*1], Tomohiro Nimura[1], Akira Murata[1] and Kaoru Iwamoto[1]*

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ABSTRACT

Pulsation control is one of promising turbulent controls for reducing skin friction drag. Significant drag reduction effect is achievable by carefully tuning pulsation parameters. However, it is difficult to optimize the pulsation control due to computational costs and the large number of parameters involved. Matsubara et al. (2023) constructed a deep learning model capable of predicting acceleration and deceleration [1], while the prediction accuracy of Reynolds shear stress (RSS) is low. In addition, its generalization capability across varying pulsation parameters remains unverified for flow fields exhibiting different drag reduction effects.

In this study, we have propose a deep learning model with a new input of RSS, building upon the framework established by Matsubara et al. (2023) [1]. The model structure comprises a convolutional autoencoder (CAE) and long short-term memory (LSTM). We normalize the low-dimensional modes obtained from CAE to enhance LSTM learning. Our training dataset consists of time series data from direct numerical simulations, including streamwise velocity, radial velocity, RSS, and pressure gradient.

It was found that the model fails to improve the prediction accuracy of RSS, although RSS is added for in training dataset. Further exploration revealed a weak correlation between low-dimensional modes and RSS. Next, we predict flow fields exhibiting various drag reduction effects resulting from changes in pulsation parameters. Interestingly, both the Matsubara et al. (2023) [1] model and our proposed model can predict these flow fields under identical parameters during both learning and prediction phases.

Investigation of prediction accuracy under different parameters during the prediction phase would reveal whether the model is predictable for flow fields with extensive drag reduction effects. This would provide valuable suggestions for improving its generalization capability.

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Computational fluid dynamics (CFD) and fluid-structure interaction (CFSI): Methods and Applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HOMOGENIZED LATTICE BOLTZMANN METHODS FOR EFFICIENT FLUID-STRUCTURE INTERACTION SIMULATIONS

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ABSTRACT

Lattice Boltzmann methods (LBM) are an established mesoscopic approach to the simulation of a diverse range of transport problems, most prominently flows described by Navier-Stokes (NSE) and reaction-advection-diffusion equations. Their algorithmic structure renders LBMs uniquely suited to massively parallel high performance computation (HPC). LBMs have successfully been used in the context of computational fluid-structure interaction (FSI), primarily by coupling external structural solvers via immersed boundary methods (IBM).

The homogenized lattice Boltzmann method (HLBM) [1] is a recent approach to modeling flows with dynamic boundaries that considers fluid and solid regions as a unified, time-dependent porous medium. The HLBM has been successfully employed for the simulation of resolved arbitrarily shaped particles [2] but remained specialized to swarms of non-deformable particles treated as discrete elements. Compared to IBM-based approaches, the HLBM offers advantages for HPC due to its local, non-interpolated nature and straightforward coupling to arbitrary structural modeling approaches.

This presentation discusses a novel approach to the simulation of arbitrary FSI problems with two-way coupled deformable boundaries using HLBM, combined with a molecular dynamics (MD) model, yielding a unified and efficient high performance FSI solver. Such a performance-focused approach is essential to enable large-scale ensemble simulations aimed at uncertainty quantification of flows derived from phase-contrast magnetic resonance imaging (PC-MRI) measurements, specifically capturing unsteady hemodynamics in moving vessels. For the present talk, benchmark results of established reference cases, including flow-induced beam bending and filament oscillation as well as an application case simulating a model of the human vocal fold will be presented. The implementation and parallel performance on heterogeneous multi-GPU clusters using the open source LBM framework OpenLB [3] will be discussed.

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Data-enhanced multi-model uncertainty quantification and experimental design of complex computational systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTI-FIDELITY SURROGATE BASED ON BAYESIAN POLYNOMIAL CHAOS EXPANSION FOR THERMOCHEMICAL NON-EQUILIBRIUM

Venkata Mridula Kuppa[*1], Roger Ghanem[2] and Marco Panesi[1]*

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ABSTRACT

Accurately predicting the surface heat flux experienced by a spacecraft during atmospheric (re-)entry is crucial for determining the appropriate Thermal Protection System (TPS) material and thickness. The high speeds involved during (re-)entry lead to the formation of strong shockwaves, beyond which flow pressure, density, and temperature rapidly increase. This results in the excitation of internal energy modes and molecular dissociation, directly impacting the surface heat flux. Modeling this phenomenon is challenging due to nonequilibrium conditions, where the characteristic time scales of species collisions become comparable to the characteristic time scales of flow.

Various models, ranging from low accuracy and low computational cost (such as multi-temperature models) to high accuracy and high computational cost (such as state-to-state models), are available to simulate thermochemical nonequilibrium. Adding to this complexity, uncertainties exist in flow parameters, such as (re-)entry speed, boundary conditions, and in chemistry rate coefficients. Accounting for these uncertainties is essential to determine the uncertainty in key quantities like surface heat flux.

In this context, the necessity for a surrogate model for non-equilibrium thermochemistry is evident, as it facilitates computationally tractable forward propagation of flow parameter and rate coefficient uncertainties. The diverse range of models at different fidelities allows the development of multi-fidelity surrogate models, leveraging abundant yet less accurate low-fidelity data and sparse but highly accurate high-fidelity data to strike a balance between accuracy and computational cost.

This work proposes a multi-fidelity surrogate model that combines numerous, less accurate low-fidelity simulations with a select few accurate, yet expensive, high-fidelity ones to create a comprehensive dataset. This combined dataset is utilized to identify a low-dimensional subspace using two methods: the linear dimensionality reduction method Principal Component Analysis and the non-linear method Diffusion Maps. Probabilistic Learning on Manifolds (PLoMS) [1] is used to enrich the high-fidelity data by conditioning on corresponding low-fidelity data. The enriched dataset is then employed to train a Polynomial Chaos Expansion (PCE) with stochastic coefficients, accommodating model form uncertainty. This multi-fidelity surrogate model, combining the strengths of dimensionality reduction and PCE, allows for quicker predictions of the full flow field at new locations in the uncertain input parameter and boundary condition space with impressive accuracy but at a significantly lower computational cost compared to high-fidelity simulations. This framework paves the way for a comprehensive characterization of uncertainty in thermochemical nonequilibrium phenomena.

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Advances in material model calibration for computational solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPARISON OF FULL-FIELD OBJECTIVE FORMULATIONS FOR MATERIAL MODEL CALIBRATION

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ABSTRACT

Critical safety simulations need to credibly model physical evolutions of their components in extreme conditions. Feature rich material models, such as those with anisotropic yield and hardening, provide the necessary physics to represent material response under these conditions. A significant obstacle in using feature rich material models is the substantial quantity of calibration parameters present. Using conventional experimental data, such as uniaxial load-displacement, to calibrate these models is difficult and requires many iterations of the same experiment. Full-field data acquisition systems and tools, such as digital image correlation and infrared cameras, provide a plethora of data from an individual experiment. Full-field data tools capture experimental measurements at a level of detail that conventional probe and fixture-based measurements cannot. Experiments designed around the capture of full-field data can enable richer sets of data from single experiments, potentially enabling the calibration of more elaborate material models with fewer experiments.

We investigate this assumption by comparing three full-field calibration techniques to a conventional calibration where only conventional data is used. The three full-field calibration techniques differ in that they provide different formulations of the objective that is minimized during calibration. The first objective studied is formed by spatially interpolating the experimental data to the simulation nodes and directly differencing the data to form a set of residuals. The second method transforms the spatial data to a common set of orthogonal basis functions, and then compares the data in this transformed space. We determine this set of basis function using a variation of Alpert wavelets[1]. The final method is an implementation of the virtual fields method [2]. In the presentation, we describe our implementation of each method and compare their performance on a set of synthetic data where the true solution is known.

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New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION FOR FRACTURE RESISTANCE USING NEURAL REPARAMETERIZATION

Gawel Kus[*1] and Miguel Bessa*[1]

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ABSTRACT

Consideration of fracture is crucial in a wide range of design problems: from simple load-bearing structures exposed to fatigue and corrosion cracks to specialized energy-dissipation designs. However, optimizing structures for fracture resistance remains one of the most complex challenges in the Topology Optimization field. The process relies on solving fracture simulations, which are expensive and challenging to combine with standard topology optimization approaches due to their non-linear nature. Furthermore, the crack trajectories are sensitive to even minor design changes, which results in a poorly behaved loss function that is difficult to optimize.

We explore addressing these challenges with neural reparameterization, where the optimization variables are represented using the latent space of a deep neural network. We investigate neural reparameterization with gradient-based and gradient-free optimizers. In the first case, we use neural reparameterization to expand the problem dimensionality, leading to overparameterization, which makes the loss landscape easier to explore by a gradient-based optimizer. In the second case, we use neural reparameterization to reduce the dimensionality of the problem to mitigate the curse of dimensionality of the gradient-free optimizer. We benchmark both methods on several examples of optimizing topology designs for fracture resistance and compare them against the conventional approach.

STRESS-STRAIN STATE OF HTSC TAPES IN SPARC CENTRAL SOLENOID

Sergey Kuznetsov[*1], Nicoli Ames[1], Jeremy Adams[1], Chris Lammi[1], Alexey Radovinsky[1], Erica Salazar[1] and Brian LaBombard[2]*

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ABSTRACT

Successful test of 20 T toroidal field model coil (TFMC) in 2021[1] demonstrated feasibility of fabrication of large scale high field HTS magnets. SPARC[2] central solenoid will be another high field, high energy HTS magnet. It is based on cable-in-conduit conductor technology. The cable consists of four twisted petals of copper former, each has a groove for a stack of soldered HTS tapes. The cable is immersed in a steel jacket, providing structural support.
During magnet operation at high field magnet will experience time-dependent electromagnetic, structural and thermal loads. Superconducting tapes will experience high mechanical stresses and strains. Exceeding certain bounds leads to degradation of superconducting tapes and reduction of critical current. At the same time, allowable stresses and strains are design specific and there is very limited information about their values for a soldered multi-tape conductor.
In this study we present multi-scale models of SPARC central solenoid and TFMC coil and estimate mechanical stresses and strains experienced by HTS tapes in both cases. We report these values and review critical stress and strain available in the literature. Based on the successful completion of TFMC test we conclude that computed stress and strain values can be considered as allowable and can be used to design new high field high energy magnets such as SPARC central solenoid.

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Predictive digital twins
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FEDERATED LEARNING FOR STRUCTURAL HEALTH MONITORING

Trond Kvamsdal[12], Adil Rasheed[12], Florian Stadtmann[1], Knut Morten Okstad[2] and Kjell Magne Mathisen[1]*

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ABSTRACT

A challenge for establishing predictive digital twins is access to data that may be confidential. Federated learning (FL) has been argued to address this issue in the context of digital twins. We show that federated hybrid models can - with the right training strategy - by design to achieve results that are of the same quality as models trained on a central data. We have combined FL with Hybrid Analysis and Modelling (HAM) to enable Structural Health Monitoring (SHM) in te context of predictive digital twins.

Numerical modelling of composite materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL MODEL FOR THERMAL BUCKLING ANALYSIS OF FGM THIN-WALLED STRUCTURES

Sandra Kvaternik Simonetti[*1], Domagoj Lanc[1], Goran Turkalj[1] and Damjan Banić[1]*

[1]*University of Rijeka*

ABSTRACT

A numerical approach for solving the problem of nonlinear stability of beam structures made of FG (functionally graded) materials under variable temperature is presented in this work. The approach utilizes a geometric nonlinear algorithm based on a 1D numerical model using a spatial beam finite element. The deformations are considered small and the Green-Lagrange deformation tensor is used for defining them. The finite element model is based on the Euler-Bernoulli beam theory for bending and the Vlasov theory for torsion. The UL (updated Lagrangian) incremental formulation is used in the nonlinear analysis with the principle of virtual works. The cross-sectional displacement field includes the effects of warping torsion and large rotations. The material properties assumed to vary continuously through the wall thickness based on power-law distribution. The proposed beam model enables buckling analysis for cases of uniform, linear and nonlinear temperature distribution through the thickness of the cross-sectional walls. The analysis also includes the temperature dependence of the mechanical properties of the material. Numerical results are obtained for different thin-walled sections with various configurations such as boundary conditions, geometry, FG skin-core-skin ratios, and power-law index to investigate critical buckling temperatures and post-buckling responses. The numerical algorithm is tested for accuracy and reliability by comparing the results obtained using 2D and/or 3D finite element models from established software packages. The comparison shows that the numerical results are in excellent agreement with the results obtained with shell and solid models.
The proposed algorithm is more efficient and faster than numerical models based on shell and solid finite elements, making it an advantage. This numerical model provides the possibility of describing and analysing beam structures made of composite FG materials during the process of their design. It is especially useful in assessing the response and loss of structural load-bearing stability in a thermal environment.

Data-driven approaches for solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NEURAL NETWORK PLASTICITY MODELS WITH ABAQUS UMAT FOR ALUMINUM 7079

Chulmin Kweon[*1], Hyoungsuk Suh[2], Brian Lester[3], Sharlotte Kramer[3] and WaiChing Sun[1]*

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ABSTRACT

This study introduces a publicly available PyTorch-ABAQUS deep-learning framework of a family of plasticity models where the yield surface is implicitly represented by a scalar-valued function. In particular, our focus is to introduce a practical framework that can be deployed for engineering analysis that employs a userdefined material subroutine (UMAT/VUMAT) for ABAQUS, which is written in FORTRAN. To accomplish this task while leveraging the back-propagation learning algorithm to speed up the neural-network training, we introduce an interface code where the weights and biases of the trained neural networks obtained via the PyTorch library can be automatically converted into a generic FORTRAN code that can be a part of the UMAT/VUMAT algorithm. To enable third-party validation, we purposely make all the data sets, source code used to train the neural-network-based constitutive models, and the trained models available in a public repository. Furthermore, the practicality of the workflow is then further tested on a dataset for anisotropic yield function to showcase the extensibility of the proposed framework. A number of representative numerical experiments are used to examine the accuracy, robustness and reproducibility of the results generated by the neural network models.

Multi-scale and machine learning-based modeling methods for optimization and design of composites
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ENHANCING THE OXIDATION RESISTANCE BY ADDING IMPURITIES TO CARBON SITE IN ULTRA HIGH TEMPERATURE CERAMICS: AN AB INITIO MOLECULAR DYNAMICS STUDY

Seunghwan Kwon[*1], Jongkyung An[1], Rajkamal Anand[1], Jiwon Jung[1] and Gunjun Yun[1]*

[1]*Seoul National University*

ABSTRACT

C/C composites are suitable structural materials for aerospace engineering because of their superior mechanical properties, lightweight and excellent thermal shock resistance, but they are vulnerable to severe degradation induced by oxidation during atmospheric reentry. Such degradation will impair their physical/chemical properties. Therefore, surface coatings are required to protect them in extreme environment. Ultra high temperature ceramics (UHTC) are promising candidates for such coatings due to their good mechanical properties and chemical stability at high temperature. However, even though we can compare the oxidation resistance of different materials experimentally, we lack the fundamental understanding of the reaction mechanisms at atomic level. In this study, we did ab initio molecular dynamics (AIMD) simulation for three types of carbides UHTC, ZrC, HfC and TaC, at various temperature and oxygen coverage. Surface orientations of each materials for the simulation were selected to (100), (110) and (111). These surface planes were selected due to their dominance of those materials, observed from the experimental results gathered from x ray diffraction or transmission electron microscopy. Moreover, we replaced carbon atom on the surface of carbides UHTC to several other elements such as B, N, O, Al, Si, P, S to further enhance the anti oxidation ability than pristine surface and executed AIMD simulation. Such doping elements were selected based on the difference in ionic radius and number of valence electrons with carbon. To substitute carbon to other elements, those should possess similar size of ionic radius and valence number. From AIMD simulation results, we gathered trajectories of each atoms and calculated diffusion coefficient of surface atoms from those trajectories to quantitatively compare the oxidation resistance of materials doped with different elements. Also, from the atomic configuration shown in snapshots, we calculated charge density difference and partial density of states to reveal the nature of chemical bonding. Further, we have gained insights about the reaction mechanisms of each materials and the effect of added impurities on oxidation based on molecular dynamics simulation trajectories that fully reflect the sequential chemical reaction process. Through this study, we were able to select the optimized impurities, enhance the oxidation resistance.

Computational fluid dynamics (CFD) and fluid-structure interaction (CFSI): Methods and Applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ACCELERATING FLUID-STRUCTURE INTERACTION SIMULATIONS WITH MULTI-TIME-STEP COUPLING OF IMPLICIT-EXPLICIT SCALAR AUXILIARY VARIABLE TIME INTEGRATION SCHEMES

Sun-Beom Kwon[*1] and Arun Prakash*[1]

[1]*Purdue University*

ABSTRACT

Simulating fluid-structure interactions (FSI) problems, such vortex-induced vibrations, is usually associated with a high computational cost because of the presence of multiple temporal scales. Most time integration schemes, however, are constrained to use the smallest time-step necessary to resolve these scales over the entire fluid and solid domain. There are several time integration schemes available to solve the Navier-Stokes equations and coupling strategies that allow fluid and solid domains to be integrated with different time-steps with different stability and accuracy characteristics. The focus in the study, however, is on recently developed implicit-explicit (IMEX) scalar auxiliary variable (SAV) schemes that are able to achieve high-order accuracy and unconditional energy stability.

In this work, we present a novel multi-time-step (MTS) method that allows the use of small time-steps in boundary layers and large time-steps in the far field to reduce computational cost while maintaining accuracy within fluid domains. Further, we formulate up to 5th order accurate IMEX-SAV schemes for structural dynamics as well and investigate different coupling strategies for FSI. We show that the proposed MTS-IMEX-SAV method for solving the Navier-Stokes equations is unconditionally stable and involves only linear algebraic systems thereby eliminating the need for iterations due to the presence of nonlinear terms. We demonstrate the computational performance of the proposed MTS-IMEX-SAV method using several numerical examples and show the computational gains compared to existing time integration schemes.

Honoring the Legacy of Prof. Patrick Selvadurai
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN IBEM-FEM MODEL OF THE CONVERSION BETWEEN SURFACE AND BODY WAVES RESULTING FROM THE INTERACTION OF PAVEMENTS WITH THE SOIL

Leonardo Antoniazzi Marques[1], David Carneiro[2], Persio Leister de Almeida Barros[1] and Josue Labaki[1]*

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ABSTRACT

This paper investigates the phenomenon of conversion of Rayleigh (surface) waves into primary and secondary body waves caused by the presence of a pavement on the soil surface. To investigate this phenomenon properly, an IBEM-FEM model is used, in which the pavement is represented via a classical finite element method (FEM) discretization, and the soil is represented via a boundary element discretization, in the context of the Indirect Boundary Element Method (IBEM). Both the pavement and the soil are modeled as linear-elastic, isotropic media, which is a reasonable model in this case, in which low magnitude, low frequency time-harmonic excitation is considered. Coupling at the interface between the pavement and the soil is achieved by establishing equilibrium and continuity conditions between the finite and the boundary element nodes of both meshes, resulting in a case in which the pavement is fully bonded to the surface of the soil. This allows for the energy exchanged between the two bodies to be represented properly as well. Because of the boundary element scheme used to represent the soil, this model can capture accurately some features of wave propagation in the soil, such as the scattering of waves due to the presence of the pavement, the conversion of surface into body waves resulting from the pavement-soil interaction, and attenuation of energy at infinity, as imposed by Sommerfeld's radiation condition. In this paper, this model was used to investigate specifically the intricated phenomenon of conversion of surface waves into body waves, especially with regards to the angle at which a wavefront of the converted body waves is injected into the soil. The results of a parametric study show how geometric and constitutive parameters of the soil and pavement affect this injection angle. Converting surface waves into body waves has shown to be one of the main mechanisms by which surface structures can be used to attenuate ground vibration. Understanding these details about this mechanism can help geotechnical engineers to design pavements that also work as ground vibration mitigation devices.

Mathematics and algorithms for predictive digital twins (DT)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NONLINEAR CFD DATA INTERPOLATION IN PARAMETERIZED ADVECTION-DOMINATED FLOWS

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ABSTRACT

The Reduced Order Models (ROM) have been introduced as a low rank approximation of a studied dynamics to speed up its evalutaion. This low rank approximation is crucial for application related to CFD as the number of degrees of freedom limits their usage in design optimization or real time evaluation for dynamics and control. Even though some ROMs have been proven efficient on certain applications, their construction around linear subspaces reduces their usage to some specific industrial cases.

To overcome this issue we propose a general interpolation technique between snapshots of parametric simulation results. The core of this method relies on the computation and the use of spatial mappings to transport the snapshots over the manifold of solutions. This kind of approach is referred to as image registration and has been largely used in medical imaging. Today we propose to apply image registration to CFD data and compute an accurate interpolation in a non intrusive manner. The method starts with the use of markers to identify the coherent structures of the flow. From these markers, we will define the registration problem as the minimisation of an energy functional depending on the mapping we are looking for. The functional is designed to fill three objectives: align the markers, produce a bijective mapping through the regularization of its displacement field and impose on the interpolation trajectories to be compliant with the boundary conditions of the CFD domain. Finally, the solution should be computed fast enough so the interpolation method remains relevant for real time applications. For this, we constructed an appropriate compact research space for the velocity of the displacement field. This research space was built as the span of the first eigenfunctions of the Navier-Lamé operator along with the appropriate boundary conditions. The regularization of the field was ensured by the minimization of its H2 norm. Finally, by applying this pseudo temporal mapping on the solution it is possible to construct non linear latent spaces [1] or use it directly to perform a convex displacement interpolation of the snapshots [2].

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Battery modeling and computation: From material to device
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL MODELLING OF LARGE POUCH LITHIUM-ION BATTERY

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ABSTRACT

The need for a reliable thermal management system for lithium-ion batteries is paramount, primarily due to the critical role it plays in maintaining an optimal operating temperature range, and mitigating aging effects. Elevated temperatures accelerate aging by increasing the rate of internal chemical reactions, leading to capacity loss and reduced battery life. To address this issue, electric vehicle (EV) battery manufacturers often employ small cylindrical cells to improve reliability and temperature uniformity, thanks to their large surface-to-volume ratio. However, this method also adds to the pack's weight, thereby affecting the vehicle's range. As a result, large pouch cells are becoming more popular in EV applications. To enhance the safety and performance of these cells, various heat dissipation techniques are employed to improve temperature uniformity and cooling. To help in the design of future large pouch cells, reliable numerical tools that can account for local temperature changes are required, moving beyond a basic single-cell model. This comprehensive method offers a more accurate simulation of real-world conditions by considering thermal variation in the electrochemical model.

A case of study in which a local thermally coupled electrochemistry model is used to simulate cell behavior and temperature variations. We investigate the design space and propose strategies to alleviate temperature non-uniformity. This approach allows us to represent and address the challenges faced in real-life applications more accurately.

Fluid-structure interaction: Methods and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATIONS OF THE PARTICLE FINITE ELEMENT METHOD FOR 3D FLUID-STRUCTURE INTERACTIONS AND MULTIPHYSICS SIMULATIONS

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ABSTRACT

The present work focuses on the partitioned coupling between a structural solver based on the Finite Element Method (FEM) and a fluid solver based on the Particle Finite Element Method (PFEM) (Idelsohn, Oñate and del Pin, 2004) in order to simulate thermo-mechanical Fluid-Structure (FS) interactions involving free surface flows and large deformations of the solid. The coupling is performed by transferring nodal information (such as the heat flux, the mechanical load, the nodal temperature and the nodal displacement) between the two solvers, under the form of Neumann-Dirichlet boundary conditions imposed at the fluid-structure interface. When the solid and fluid meshes are non-matching at the interface, an interpolation technique is required to transfer the nodal data from one solver to another. In particular, the Radial Basis Function (RBF) interpolation is considered for its flexibility and its efficiency (Lacroix et al. 2024).

The use of different solvers aims at combining their individual potentials for simulating complex physics (such as phase change and free-surface flows on the fluid side, or rupture and contact mechanics on the solid side) while exchanging a minimum amount of information between the two solvers to achieve the coupling (Cerquaglia et al. 2019). The presentation starts with a brief introduction to the basic principles of the PFEM and the Neumann-Dirichlet partitioned coupling, followed by a discussion regarding the mesh-interpolation technique. Notably, the interpolation step and the detection of the FS interface is challenging when the boundaries of the fluid and of the solid evolve in their topology due to large deformations, rupture of finite elements or local mesh refinement. Finally, our presentation includes some examples of applications of the FPEM in friction melt bonding, water-jet cutting or frictional contact between debris in a pipe.

Advances in multi-scale, multi-material, and multi-component Topology Optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION FOR THE DESIGN OF MANUFACTURABLE PIEZOELECTRIC ENERGY HARVESTERS USING DUAL-MMC METHOD

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ABSTRACT

A new topology optimization scheme for the manufacturable piezoelectric energy harvesters (PEHs) are proposed. Most of the existing topology optimization schemes for the design for PEHs are difficult to cope with manufacturing constraints producing design results that pose serious challenges for the local poling of the piezoelectric materials. In this work, dual-Moving Morphable Component (dual-MMC) scheme for explicit topology optimization for the design of PEHs is presented. In dual-MMC scheme, two independent sets of MMC are employed to describe the structural topology of the PEH and polarization profile in piezoelectric material in an explicit manner. With the use of the scheme, the shape of electrodes and the opposite polarization directions in the local poling process can be effectively treated as a constraint making the realization of the PEH an easy task. Several examples for the design of cantilever-type PEH are provided to demonstrate the effectiveness of the proposed approach. Furthermore, a designed PEH is actually manufactured to demonstrate of the production process.

Fluid-structure interaction: Methods and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN UPDATED LAGRANGIAN PARTICLE HYDRODYNAMICS (ULPH) - NON-ORDINARY STATE-BASED PERIDYNAMICS COUPLING APPROACH FOR MODELING FLUID-STRUCTURE INTERACTION PROBLEMS

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ABSTRACT

In order to solve the fluid-structure interaction problem of Newtonian fluid, a fluid-structure interaction approach is proposed based on Non-ordinary State-based Peridynamics (NOSB-PD) and Updated Lagrangian particle Hydrodynamics (ULPH), to simulate the fluid-structure interaction problem in which large geometric deformation and material failure are considered. In the coupled framework, the NOSB-PD theory is used to describe the deformation and fracture of the solid material structure. ULPH is applied to describe the flow of Newtonian fluids due to its advantages in computational accuracy. The framework effectively utilizes the advantages of NOSB-PD theory for solving discontinuous problems and ULPH theory for solving fluid problems and has good computational stability and robustness. To deal with the interface of fluid structure, a fluid-structure coupling algorithm using pressure as the transmission medium is established. The dynamic model of solid structure and the PD-ULPH fluid-structure interaction model involving large deformation are verified by several numerical validations, which are in good agreement with the analytical solution, the available experimental data and other numerical results, that demonstrates the accuracy and effectiveness of the proposed method in solving the fluid-structure interaction problem. Overall, the fluid-structure interaction model based on ULPH and NOSB-PD established in this paper provides a new idea for the numerical solution of fluid-structure interaction and a promising approach for engineering design and experimental prediction.

Modeling and simulation of coupled processes in geological media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADVANCING GRANULAR MATERIAL ANALYSIS: NEURAL NETWORK-DRIVEN REPRESENTATION AND COMPUTATIONAL PARTICLE MECHANICS VIA SIGNED DISTANCE FIELDS

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ABSTRACT

We introduce a novel approach, the Neural Network-Encoded Signed Distance Field (NetSDF), for the representation of shapes and computational particle mechanics in granular materials. Our method utilizes a neural network to learn and depict a Signed Distance Field (SDF), which defines a mapping from a point to a signed distance. Specifically, the neural network takes point coordinates and a latent code representing a single shape as inputs, generating the signed distance from the point to the particle surface. The sign distinguishes between the interior and exterior of a particle, making the zeroth isosurface of the SDF an accurate representation of the particle surface. Upon training the NetSDF with a designated set of particle samples, it can effectively represent an entire class of particles exhibiting the characteristic morphology of the granular material. Our results demonstrate the NetSDF's proficiency in accurately representing irregular-shaped particles and generating virtual particles within the same class. Moreover, the NetSDF seamlessly integrates with the SDF-based discrete element method (Lai et al., 2022, Computational Mechanics), showcasing notable advantages in terms of memory consumption and computational efficiency.

Advanced numerical methods for the modeling and optimization of coupled dynamical systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING OF AN OBLIQUE INCIDENT P-WAVE WITHIN A WATER SATURATED SOIL WITH THE WAVE BASED METHOD

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ABSTRACT

Due to irregularities at the surface of a soil, oblique incident wave fronts may cause amplifications of displacements and stresses. To model these for a water saturated soil in the 2D case, it is necessary to consider two irrotational potentials (1st and 2nd P-wave) and one solenoidal potential (S-wave). The Wave Based Method (WBM) permits to model poroelastic soil for a harmonic loading efficiently, which has already been shown for a surface loading [1]. The following contribution focusses on the modeling of an incoming 1st P-wave, which excites a poroelastic halfspace with a trapezoidal canyon.

Amongst other advantages of the WBM, this numerical method is chosen as it needs significantly less degrees of freedom than a finite element approach to model a boundary value problem. This saves computational time, especially for the approximation of an infinite poroelastic soil medium.

In this contribution, a coupling approach between the WBM and an oblique incident 1st P-wave is presented. The approach is used to model a poroelastic halfspace with an empty canyon. The system’s response is compared with a reference solution from literature. Moreover, a second coupling approach is introduced to permit the modeling of a filled canyon. In the special case of a canyon filled with the material of the surrounding soil, the simulation results are compared with the underlying analytical solution.

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Complex fluid flows in engineering: Modeling, simulation, and optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ON THE DESIGN OF CONFORMAL COOLING CHANNEL THROUGH TURBULENT FLOW TOPOLOGY OPTIMIZATION

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ABSTRACT

Research on improving the efficiency of heat exchangers has been a longstanding focus, impacting not only the heat exchanger industry but also extending to areas like the mold and die sector. In molding processes, the material cooling time is often the bottleneck when aiming to reduce the part cycle time. Traditional straight-line drilling often leads to suboptimal cooling, particularly in overheating-prone areas. To enhance the tooling's performance and sustainability, the use of conformal cooling channels is a promising solution, especially in processes like aluminum die casting. However, the design of conformal cooling lines in mold inserts can become particularly complex, especially when the cast part involves intricate features such as deep ribs or elongated cores. This work focuses on the application of topology optimization for conformal cooling channel design in a simplified mold geometry. Our framework employs a porosity-based conjugate heat transfer model and considers turbulent flow conditions through the use of a linear eddy viscosity model. The topology optimization algorithm aims at improving the overall cooling performance of the insert, which here translates into a balance between maximizing heat dissipation and ensuring uniform temperature across the cavity surface. The latter is achieved by penalizing the objective function with the surface temperature standard deviation. A projected-perimeter-based additive-manufacturing constraint is further employed to limit the generation of overhangs. One sub-objective of the investigation is to assess the cooling efficiency of the designed channels in comparison to a counterpart optimized for laminar flow conditions. Lastly, to validate the computations, dedicated experiments are conducted using an additively-manufactured prototype based on the optimized cooling channels design.

Continuum biomechanics of active systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HYBRID KNOWLEDGE- AND DATA-DRIVEN LIVER SIMULATION ON MULTIPLE SCALES

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ABSTRACT

The liver, a crucial organ for metabolic functions, exhibits a complex interplay between perfusion and function across multiple scales, from the entire organ to microscopic liver lobules and cellular structures. To unravel the complex hepatic function-perfusion relationship, we present a novel multicomponent, poroelastic multiphase, and multiscale function-perfusion model based on the Theory of Porous Media [1,2].

At the lobular scale, our model incorporates a homogenized tetra-phasic mixture body, representing healthy liver tissue, blood, and growing and depleting solid phases mimicking fat and tumor tissue. On the cellular scale, systems biology models express metabolism as well as metabolite production, utilization, and storage within liver cells. Bridging to the whole-body scale, interactions with organs like the kidney or lung are integrated.

To achieve seamless multiscale coupling, we employ a modular and efficient tri-scale ODE-PDE-ODE coupling approach. This framework enables simulations of critical processes such as detoxification, zonated fat accumulation, and ischemia-reperfusion injury during transplantation [2].

In a step toward clinical applicability, we enhance the model using hybrid knowledge- and data-driven approaches. Realistic liver lobule geometries are derived from histological sections, enhancing the model's accuracy. Additionally, patient-specific data provided by clinical partners enrich the simulations, allowing for individualized analyses of hepatic processes [3].

This integrated approach not only advances our understanding of the hepatic function-perfusion relationship but also provides a powerful tool for predicting and optimizing outcomes in clinical scenarios. In perspective, such a computational model can serve as a clinical decision supporting tool.

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[2] Lena Lambers, Multiscale and multiphase modeling and numerical simulation of function-perfusion processes in the liver Dissertation (2023)
[3] B. Christ et al., Hepatectomy-induced alterations in hepatic perfusion and function - toward multi-scale omputational modeling for a better prediction of post-hepatectomy liver function, Frontiers in Physiology 12 (2021), 733868

Advanced multiscale and adaptive numerical methods for non-linear solids
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A HIERARCHICAL QUADRATURE ELEMENT METHOD FOR TWO- AND THREE-DIMENSIONAL GEOMETRICALLY NONLINEAR ANALYSES

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ABSTRACT

High-order finite element methods have the advantages of fast convergence, insensitiveness to mesh distortion, and convenience to realize adaptive analysis. As a high-order scheme, the hierarchical quadrature element method (HQEM) has already been applied to linear finite element analysis and was found to be with high accuracy and efficiency. Under the constant stiffness assumption, the solution equation of stiffness only needs to be constructed and solved once, without any updating when the structure is deformed, which greatly simplifies the calculation. However, for many practical applications in engineering, such as in aerospace applications, it is unrealistic to assume constant stiffness and must be considered as nonlinear. Geometrically nonlinear analyses require repeated iteration and updating of the stiffness matrix. This paper carries out geometrically nonlinear analyses of two-dimensional (2D) and three-dimensional (3D) configurations using the HQEM under the total Lagrange framework. Based on the Green-Lagrange strain tensor and the second Piola-Kirchhoff stress tensor under the reference configuration, the virtual work equation is constructed and discretized in the space domain. In this work, the quadrilateral element is formulated for analyzing large deformation problems in plane stress, and hexahedral element is developed for analyzing geometrically nonlinear problems in complex spatial three-dimensional structures such as spatial beams and shells. The static analysis problem of unidirectional load increase can be solved by Newton-Raphson method, and the analysis of post-buckling characteristics can be solved by arc-length method. The results of several typical examples obtained by HQEM were firstly compared with the widely verified reference results to verify the correctness and accuracy of HQEM, and then compared with commercial software Abaqus to verify its high efficiency. Compared with low-order schemes, HQEM requires far fewer degrees of freedom when analyzing the same problem. It shows that HQEM has a promising application prospect in geometrically nonlinear analyses.

Computational fluid dynamics (CFD) and fluid-structure interaction (CFSI): Methods and Applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE EFFECT OF THE DIAMETER OF THE LAUNCH CANISTER ON THE SHAPE OF THE CAVITATION OF THE VEHICLE

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ABSTRACT

In this paper, the effect of the change of the diameter of the launch canister on the shape of the tail cavitation bubble generated during the salvo discharge of the vehicle is studied.
The research method was a combination of experimental and simulation research, and the Monte Carlo algorithm was used to estimate the cavitation area and then analyze.
In terms of experimental research, a launch system with variable diameter of the launch canister was established, and the salvo test was completed with a high-speed camera, and the tail cavitation morphology and motion trajectory images recorded by the twin-engine vehicle in the hydrostatic launch test were first observed, and the flow field interference between the two launchers and their tail cavity morphology were analyzed during the salvo out of the water, and the influence of the diameter of the launch canister on the salvo was analyzed.
In terms of simulation research, a simulation model of the six-degree-of-freedom motion of the salvo water was established, and the underwater salvo simulation with different launcher diameters was carried out accordingly. For the cavitation morphology of the vehicle under different working conditions, the Monte Carlo algorithm is used to estimate the cavitation area, and the variation law of the cavitation of the vehicle with the diameter of the launch canister is given, and the reasons for the area change are analyzed.

Current trends in phase-field modeling and computations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A PHASE-FIELD VISCOELASTIC MODEL FOR THE DESCRIPTION OF CRACK PROPAGATION IN ELASTOMERS

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ABSTRACT

The experiments on fracture dynamics in pre-stretched elastomeric membranes proposed in [1] have shown that crack propagation speed is proportional to the amount of pre-stretching applied to the membrane. Additionally, the numerical analysis performed in [2] has shown that the evolution of crack is influenced by the viscous dissipation occurring in the material surrounding the crack tip.
In this talk, a mechanical model for the description of crack evolution in elastomers is proposed, which is able to capture the main features of fracture dynamics observed in experiments [1,2]. A variational theory for finite viscoelasticity is formulated that incorporates phase-field fracture. Besides the viscosity related to strains, a viscous force driving the fracture is included. Consequently, two distinct characteristic times appear into the formulation which influence both the advancement of the crack and the relaxation of strain in the material close to the crack tip.
The rule played by the two characteristic times on the crack evolution is investigated through analytical estimates and numerical simulations.

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GENERALIZED HILL-MANDEL-CONDITION FOR DISSIPATIVE POLYCRYSTALLINE FERROIC MATERIALS

Stephan Lange[1] and Andreas Ricoeur*[1]

[1]*University of Kassel*

ABSTRACT

The class of so-called smart materials nowadays ranges from magnetostrictive and shape memory alloys to electro- or magnetoactive polymers and ferroelectrics. As components of smart structures, this class of materials is widely used in different fields of application, e.g. the automotive sector, in the field of medical engineering or in the aerospace technology. Thus, the modeling of the constitutive behavior of smart materials has been in the focus of solid mechanics for more than 30 years. Approaches are basically divided into phenomenological and micromechanical/-physical ones. The problem of many, in particular phenomenological constitutive models, is the comparatively large number of parameters, typically exceeding the number of key quantities available from experiments. Consequently, the fitting does not yield a unique set of parameters, thus allowing for a certain arbitrariness. Micromechanical models, on the other hand, are mostly restricted to switching within a crystallographically defined set of domains of a single grain or consider polycrystalline behavior with unconstrained reorientation of an arbitrary number of domains, suitable to represent changes of macroscopic polarization.

With the so-called condensed method (CM) a different approach has been introduced to model the constitutive behavior of ferroelectrics [1, 2]. The latter involves processes on different scales with a focus on transition from grain to polycrystalline level, considering mechanical and electric intergranular interactions. The aim of this talk is the derivation of a generalized Hill-Mandel-condition for dissipative polycrystalline ferroic materials. In [3] an extension of the classic Hill-condition towards linear piezoelectric materials was introduced. It could be proven that the generalized condition was fulfilled, independent of the control volume, by assuming homogeneous stress or strain and electric field or electric displacement. First, it is reviewed, if the generalized condition holds for nonlinear ferroelectric materials, too. Since this is not the case, it is proven under which conditions the generalized Hill-Mandel-theorem is fulfilled for dissipative polycrystalline ferroelectric material behavior. The findings can be generalized and applied to other ferroic materials and beyond and provide a framework for energetically consistent multiphysical scale transitions.

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Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DAMAGE THRESHOLD AND LIFETIME PREDICTION FOR MULTIAXIAL CYCLIC LOADING

Kai Langenfeld[*1], Rodrigue Desmorat[2], Patrick Kurzeja[1] and Jörn Mosler[1]*

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ABSTRACT

The accurate prediction of fatigue-induced failure remains an essential task in engineering. When considering metals subject to low cycles fatigue, failure typically develops in two phases: (i) the nucleation phase and (ii) the coalescence phase. Cracks nucleate at the micro scale due to cyclic plastic deformation, which subsequently coalesce into cracks at the macro scale, cf. [1]. Nowadays, numerous models exist in order to predict the lifetime of components and structures subject to cyclic loading. For instance, critical plane approaches are an efficient tool for the prediction of the lifetime with respect to uniaxial load paths [2]. For multiaxial load cases, however, continuum damage mechanics might be more accurate to consider the interaction between different strain component. Within the respective models, the criterion for damage initiation is of utmost importance.

The probably most frequently damage initiation criterion in the spirit of continuum damage mechanics is based on the stored energy function [1]. An extended initiation criterion has been proposed, which additionally accounts for the plastic strain amplitude to distinguish between different load amplitudes on the local scale [3].

The present talk focuses on the formulation of a new damage initiation criterion suitable for multiaxial fatigue – e.g., cyclic tension and cyclic torsion. As a first step, a constitutive model suitable for ductile material degradation will be extended to account for the different mechanisms associated with multiaxial loading. Subsequently, the damage initiation criterion in [3] will be modified. To be more precise, the inclusion of additional stress/strain invariants allows to explicitly account for the degree of multiaxiality. The capabilities of the extended criterion will be demonstrated by means of fatigue experiments. It will be shown that this extension can indeed capture failure associated with multiaxial
cyclic loading.

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Imaging and computational methods for biomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MONOLITHIC TWO-LEVEL SCHWARZ PRECONDITIONERS FOR MICRO-MACRO HETEROGENEOUS BLOOD FLOW

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ABSTRACT

In this talk, a machine learning-enhanced multiscale approach for the simulation of blood flow is presented. In the computational framework two different scales are combined: a macroscopic scale that models blood as a non-Newtonian continuous fluid and a mesoscopic scale that captures the behavior of red blood cells within the flow. Specifically, we aim to enhance the mass and momentum balance laws of classical continuum mechanics by using a data-driven approach leveraging data from cell-resolving mesoscopic simulations. Efficient parallel finite element solvers allow for the simulation of blood flow in complex and large geometries. More precisely, monolithic overlapping two-level Schwarz domain decomposition methods with GDSW coarse spaces are used to iteratively solve the macroscopic problem in parallel. Here, the implementations from the solver package FROSch (Fast and Robust Overlapping Schwarz), which is part of Trilinos, are used. The numerical properties as well as the parallel scalability of the solver applied to the micro-heterogeneous non-Newtonian flow problems are discussed.

Advances in computational mechanics for flow-induced vibrations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SPARSE SENSOR DATA-DRIVEN DIGITAL TWIN FOR PREDICTION AND ESTIMATION OF GOVERNING EQUATION OF A PIPE-CONVEYING FLUID USING UNSCENTED KALMAN FILTER

Vincent Laperle[1], Esmaeil Ghorbani[1] and Frederick Gosselin[1]*

[1]*Polytechnique Montréal*

ABSTRACT

This study presents our findings toward building a sparse sensor data-driven digital twin (DT) with various time integration approaches. Specifically, we evaluate the performance of Unscented Kalman filter (UKF) for predicting states and estimating parameters of any underlying system with sparse measured vibration data. The UKF is a two-stage iterative process that comprises a prediction phase and an update phase to identify the governing physical equation of the mechanical system. However, the predictions and estimation of the method can be compromised as the number of unknowns increases. The latter is a bottleneck for identification of complex mechanical system, such as hydroelectric turbines generating units. Furthermore, for data-driven DTs, the accuracy of estimation is correlated to the quality and sampling rate of the sensor data, which is the main concern of this study. To achieve this, we chose several well-known numerical models as case study to assess the performance of the UKF with different sampling rates in a decreasing scheme. Moreover, we change the time integration scheme and evaluate the performance of the UKF using the same sparse data. In this work, Heun's method is used as the main time integration scheme and will be compared to the Euler method, currently used in the classical UKF, as well as to a fourth-order Runge-Kutta (RK4) method. Model verification is accomplished by comparing UKF predictions and estimates with the actual analytical response of the mathematical model. The primary objective of this work is to identify and quantify the threshold between sensor sampling rate and model response accuracy using our UKF. We plan to validate the model in real time on a pipe conveying fluid system. The UKF model will be used to estimate defects and imperfections of the pipe-conveying fluid experiment, as well as estimate the operating conditions based on sensor measurements. The pipe conveying fluid system is an interesting model for digital twin developments because of its relative simplicity combined with the richness of the dynamics it exhibits: buckling and flutter instabilities, flow-added damping, limit-cycle oscillations, period doubling, chaotic motion, etc. Through this laboratory scale demonstration of a digital twin, we seek to demonstrate tools that could be adapted to full-scale hydroelectric power generating units.

Keywords: Data-driven digital twin, Sparse sensor data, Unscented Kalman Filter, Pipe-conveying fluid, fluid-structure interactions

VARIATIONAL PHASE-FIELD FRACTURE WITH CONTROLLED NUCLEATION

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ABSTRACT

We briefly review the Gamma-convergence of phase-field fracture to Griffith fracture, and describe how softening and nucleation occur when implementing phase-field models. An example is given of how this softening and nucleation can be completely stopped, while preserving crack growth and Gamma - convergence (crack growth can also be stopped). We then show how nucleation can locally be turned back on, based on any criterion, such as a stress threshold. Again, all modifications preserve Gamma-convergence, and they can be applied to static, quasi-static, and dynamic models. Additionally, we describe why these modifications can be expected to improve the convergence of phase-field models.

Immersed-boundary variational methods: Theory, data structures, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

WEAK AND STRONG STABILISATION OF CUT FINITE ELEMENT METHODS

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ABSTRACT

Cut finite element methods are based on embedding a computational domain into a background mesh that is not required to match the boundary. This leads to so-called cut elements at the boundary. By adding stabilization terms, we can control the variation of the discrete functions close to the boundary. This allows us to prove stability, condition number estimates, and optimal order a priori error estimates. Alternatively, we may use a discrete extension operator and solve the problem in a subspace of the finite element space where the unstable degrees of freedom are eliminated to retain optimal order approximation bounds. These two approaches, the first weak and the second strong, have the same goal: stabilizing the method, but they appear very different at first glance.

In this talk, we show that the definition of stabilization terms, added to the weak statement, may be generalized in two ways: (1) The stabilized quantity may be some functional of the discrete function, for instance, finite element degrees freedom. This allows us to stabilize the unstable modes more precisely than standard approaches, which may be considered element-based. (2) The choice of elements that are connected. Typically, face neighbors or connected patches are used, but we may stabilize by connecting elements intersecting the boundary to an element within a distance proportional to the mesh parameter. We show that the generalized stabilization form fits into the standard abstract requirements, and as a consequence, we obtain stable and optimal order convergent methods for second-order elliptic problems.

We also show that for a robust design of the ghost penalty, one may let the stabilization parameter tend to infinity without introducing locking. The limit corresponds to strong enforcement of certain algebraic constraints, identical to constraints implemented in specific extension operator frameworks. This illustrates the very close connection between stabilization and extension approaches.

Certification of simulations and model adaptation in computational science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

REDUCED ORDER MODELING WITH ERROR CONTROL FOR APPLICATIONS IN COMPUTATIONAL HOMOGENIZATION OF POLY-CRYSTALS

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ABSTRACT

Computational homogenization for finite element analyses is a multiscale framework, where the microscale features are accounted for in the (homogenized) macroscopic problem through explicit modeling of the underlying microscale on Representative Volume Elements (RVEs). More specifically, the macroscopic response is defined through the pertinent boundary value problem of an RVE. In a so-called “finite element squared” (FE2) procedure, this introduces an RVE problem associated with each macroscopic quadrature point. Such an approach becomes prohibitively expensive when the macroscale problems represent engineering structures/components. Reduced Order Modeling (ROM) is associated with the aim to reduce the computational cost when a similar problem is solved numerous times for slightly different data. The solution to the RVE-problems, where we typically seek the effective response for large variety of different macroscopic kinematic histories, is a perfect example of a problem suitable for ROM.

In this contribution, we consider the applications of polycrystals, where each grain is modeled using (gradient enhanced) crystal plasticity. A reduced order basis is constructed, using Proper Orthogonal Decomposition (POD), in terms of the dissipative stresses associated with the inelastic slip fields. Based on linear kinematics, the corresponding displacement and slip fields associated with the basis can be computed at an offline stage. Ultimately, the online evaluation of the macroscopic stress-strain response is obtained by use of a Galerkin projection method for the adopted basis. For the reduced order model, controlling the error in terms of the effective macroscopic response is imperative. To this end, we investigate a few different error estimators of varying computational cost. The accuracy and computational efficiency of the proposed ROM, as well as the performance of the different error estimators are investigated for a few basic numerical examples.

Verification techniques in computational physics and applied mathematics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

WALL-MODELED LARGE EDDY SIMULATION OF SMOOTH-BODY SEPARATION: RESULTS OF A CFD VERIFICATION WORKSHOP

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ABSTRACT

The talk will summarize the lessons learnt from the authors' participation in the AIAA High Fidelity CFD Verification workshops held in 2022 and 2024, with a focus on the smooth-body separation test case. The test case features a fully developed incoming turbulent boundary layer at a Reynolds number that is sufficiently large to warrant the use of a wall-model, and a smooth backward-facing ramp that causes a large separation bubble. Participants had to submit blind predictions for this case, with an emphasis on the convergence of the results during grid-refinement.

The results show how elusive grid convergence can be for this type of problem, with most solutions failing to show convergence even on grids with many hundred million elements. The issue of of converging averages and the computational demands it imposes on separated flows will also be discussed, with implications on verification. The talk will also discuss several numerical experiments aimed at elucidating which simulation parameters most strongly affect the results, including the incoming turbulent boundary layer, the spanwise domain width, details of the numerical method, and details of the computational grid. In addition, experiments with residual evaluation as a means to judge where in space errors are introduced will be discussed.

MODELLING ROCK CUTTING TRANSPORT BY A COUPLED BONDED PARTICLE MODEL AND CFD

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ABSTRACT

To understand the fracture of rock materials and the subsequent transport of rock cuttings by fluid is of fundamental importance for efficient rock drilling. The industrial incentives are many. For instance, an estimated 50 % of the total cost per installed megawatt geothermal energy is associated with drilling and well construction [1]. Multiphysics simulations provide a means to improve knowledge and understanding of rock drilling, including rock fracture, transport of cuttings and wear on drilling equipment.

In the present study, a Multiphysics approach for modelling rock drilling and transport of cuttings by fluid is proposed. The rock material is modelled by a recently developed statistical bonded particle model (BPM) [2,3]. In the BPM, rock heterogeneities are included by using statistically distributed grain sizes and shapes as well as Weibull distributed mechanical properties. The drilling fluid is modelled by computational fluid dynamics (CFD) based on the particle finite element method. The transport of cuttings during rock drilling is modelled by coupling the BPM and CFD models. Coupling of the models is realized by a loose (or weak) two-way coupling strategy.

By the coupled BPM-CFD models, the complex dynamics inside the drill hole are predicted. The model is used to quantify drilling rate of penetration, mass of transported cuttings and fluid flow in the drill hole.

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Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPETITION OF CRAZING AND SHEAR YIELDING UNDER CYCLIC MODE I LOADING USING A MOLECULAR DYNAMICS INFORMED CONTINUUM MICROMECHANICAL CRAZING MODEL

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ABSTRACT

Shear yielding and crazing are the key deformation and damage mechanisms which govern the inelastic behaviour of glassy polymers. The present work studies the interaction of both mechanisms during crack growth under cyclic mode I loading. To this end and as primary aim of this work, a continuum micromechanical crazing model for cyclic loading conditions has been developed [1]. To further elucidate the crazing process on the molecular level, molecular dynamics simulations of a carefully equilibrated coarse-grained bead-spring model are used to study the fibrillation process and the response of craze fibrils under cyclic loading. This is in contrast to previous work, which focused solely on monotonic loading conditions (e.g. [2]). With insights from these simulations, the continuum model is subsequently refined, resulting in a more realistic molecular dynamics informed constitutive model for crazing. This model is then applied along the ligament of a mode I boundary value problem to investigate craze and crack propagation in glassy polymers. The deformation in the glassy bulk material is described by the well-established constitutive model by Boyce and co-workers (e.g. [3]) which accommodates shear yielding. This approach allows to effectively model and study the interplay between crazing and shear yielding under cyclic loading conditions.

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Multiscale Theory and Modeling of Advanced Nanocomposites
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEGRADATION OF GLASS FRP IN MARINE ENVIRONMENT

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ABSTRACT

Glass fiber reinforced polymer (FRP) has been widely utilized in marine applications due to its excellent performance in the application of seawater sea-sand concrete. Although many experimental investigations have been carried out to determine the characteristics of the glass FRP under various experiments, in-depth insight into molecular-scale processes involving interfacial interactions between fiber and matrix cannot be provided. Therefore, modeling under atomistic and mesoscale is necessary so as to understand the origin of material degradation initiated from the material interface. The multiscale modeling framework that includes both molecular dynamics simulations and coarse-grained (CG) models beyond the capacity of atomistic simulations has been put forward. In this work, the degradation mechanism of glass FRP in hygrothermal and chloride environments is indicated through the changes in material structure, decreased adhesion energy, reduced interfacial stress, and the weakened intermolecular interactions with the consideration of hydration bond. The performance of different degraded polymer matrices is also compared. The work provides fundamental information on interfacial deterioration in glass FRP, which can be further extended to the research on deterioration of other engineering composite materials and the development of new nanocomposites.

Multi-physics and multi-scale simulations with the coupling library preCICE
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GISMO & WATERLILY ADAPTERS FOR THE PRECICE COUPLING LIBRARY

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ABSTRACT

Fluid-structure interaction occurs in a wide range of fields of science and engineering, from biomedical to aerospace. It covers problems such as aortic valves and bristled wings. The potentially large-scale separation between the two sub-problems makes it difficult to derive general monolithic approaches. Partitioned approaches avoid this issue by allowing problem-specific solvers for each sub-problem and coupling them through the boundary conditions. In recent years, the preCICE library [1] has greatly improved the possible solver combination to tackle these problems.
Here, we present two new adapters for the preCICE coupling library that allow the simulation of strongly coupled, geometrically non-linear, fluid-structure interaction problems. We follow the standard Dirichlet-Neumann approach; we coupled both solvers through the interracial displacements and stresses. Using the direct mesh access of preCICE, we couple a finite-volume immersed-boundary fluid solver, WaterLily.jl [2], to an iso-geometric structural solver G+Smo. Using immersed boundary and iso-geometric analysis allows for arbitrary interface displacements within the fluid solver. Nurbs-based representation of the structure within the fluid solver allows for analytical distance function and normal vector. The iso-geometric approach for the structural problem significantly improves basis function continuity and reduced element count. This ultimately results in a fast and accurate coupling approach.
We demonstrate the capabilities of the adapters by performing 2D and 3D simulations of complex fluid-structure interaction systems. We focus on membrane and plate/shell structures with a perpendicular flap, inverted flag, and flapping filaments. We also demonstrate that the coupled solver is agnostic to the structural model (Euler-Bernoulli beam, Kirchhoff-Love shell). Finally, we discuss the GPU acceleration of the fluid solver and the effects on the resulting coupled solver.
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Extended digital twins including uncertainty and complexity of human/society and human knowledge
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SIMPLIFIED MAINTENANCE ACTIONS FOR INDUSTRIAL DECISION SUPPORT SYSTEMS

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ABSTRACT

Introduction: Decision support systems (DSS) used in industrial predictive maintenance encounter the challenge of distinguishing relevant from irrelevant information for user recommendations. This challenge becomes more pronounced as the number of available maintenance actions increases, leading to a dense decision network of possible actions. To reduce the number of decisions, we can remove similar decisions from being used in a DSS, leaving only distinct decisions.

Methods: We define similarity of maintenance decisions as a function of cost of taking a repair action vs the result of taking a repair action. Using a sample case in Nuclear Plant maintenance, we set Time To Repair (TTL) as the cost of taking a repair action and Remaining Useful Life (RUL) in years as the result of taking a repair action. We generated 4 datasets of random repair actions that conforms to a monotonic relationship between TTL and RUL. In this sample case, we used SCARLET (Similarity-based Clustering and Reduction of Action pLans for Effective Decision SupporT), a novel algorithm, to reduce the number of redundant maintenance actions by eliminating the most divergent actions within similar pairs. SCARLET also avoids removing action pairs that are exist on opposite sides of the threshold border. This process iterates until no redundant actions remain.

Results: When reducing actions to a manageable size (n<100), our findings revealed that SCARLET achieved between 2% to 15% error across datasets of varying sizes. In the accuracy test, we confirmed that SCARLET’s ability to classify redundant actions against domain knowledge of cost (TTR=2) and result (RUL=1.08) thresholds was high, achieving an AUC of >80% compared to other rival methods (<80%).

Discussion: SCARLET's unique approach of leveraging similarity-based clustering enables it to identify and eliminate redundant information against domain-knowledge, resulting in a more compact and representative dataset which considers of cost and result thresholds. Through the result, we see that in borderline cases where actions exist within cost and result thresholds, SCARLET is the most effective approach to take as the algorithm handles cost and result thresholding.

Conclusion: By avoiding the incorrect removal of non-redundant data, SCARLET, compared to other conventional techniques, has a more domain driven reduction approach in special borderline cases where actions exist close to cost and result threshold borders. The result of this study is important for the development of human understandable, and accurate decision-making systems by removing unnecessary decisional nodes in a dense network.

CONSTRAINED PARAMETRIC GLOBAL OPTIMIZATION OF A VIBRATION PROBLEM WITH NON-LINEAR INTERFACES

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ABSTRACT

The design of complex structures is a challenging task, especially for structures with non-linear interfaces. In this context, the use of advanced numerical methods is required to accurately predict the behavior of the structure. However, these methods are often computationally expen sive, which makes the global optimization of such structures difficult especially when classical optimizers are used. In this work, the considered vibration mechanical problem, which remains on the design of an anti-tipping device for a gantry crane [1], is solved using Craig-Bampton and a Harmonic Balance Method [2] improved with Alternating Frequency-Time approach [3] and continuation procedures. This strategy allows to compute the response along a frequency range and for a set of design parameters which govern, here, the non-linear behavior at the inter- faces (stiffnesses and gaps at contact area). Although the approach provides accurate solutions with a significant time reduction in comparison with other approaches (time iterative solver for instance), this method remains computationally expensive and not suitable for constrained global optimization. Therefore, a constrained Bayesian optimization is used to find the optimal design of the structure. Based on Gaussian Process, this method consists in the construction of initial surrogate models for the objective and constraint functions which are iteratively infilled with new responses in order to efficiently locate the optimum. For this purpose, an acquisition function called Constrained Expected Improvement is used. The proposed strategy is applied on the gantry crane problem and it is especially analyzed for many number of initial sample points. It shows good performance to identify optimal design with a limited number of solver calls.

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Recent advances in computational fracture mechanics and failure analysis
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DAMAGE IN CONTINUUM-KINEMATICS-INSPIRED PERIDYNAMICS

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ABSTRACT

Peridynamics (PD) is a nonlocal continuum formulation that was introduced by Silling in 2000 [1] and has become more and more established in the field of fracture and damage mechanics. The PD balance equations are governed by an integral term which computes the interactions between a continuum point and its neighboring points within a finite distance. Modeling damage therefore no longer leads to singularities as partial differential equations are replaced by integral terms. The basic version of PD, i.e., bond-based PD, is restricted to a fixed Poisson ratio, since it lacks the consideration of volume dilation. Recently, Javili et al. [2] have overcome this limitation by transferring the kinematic measures of CCM to a nonlocal setting, resulting in a geometrically exact theory, called continuum-kinematics-inspired peridynamics (CPD). There, in addition to pair-wise interactions, multi-neighbor interactions characterize the interplay of points. In this manner, it is possible to capture changes in length through one-neighbor interactions, changes in area through two-neighbor interactions and changes in volume through three-neighbor-interactions. The novelty of this work is the introduction of damage into the formulation of CPD. For each type of interaction, we introduce a separate damage variable, ranging from 0 for an intact interaction to 1 for a fully damaged interaction. The damage variables are obtained by evaluating a damage function at the current length strain, area strain and volume strain, respectively. An interaction is considered fully damaged once a critical threshold is reached. The choice of the damage function allows to model not only abrupt damage but also progressive damage. The latter is achieved by modeling a gradual decrease of the interaction forces until they are completely deactivated. Examples are linear, exponential and power law decreases of the interaction forces (see [3]). In this work, the proposed damage model is presented in detail and investigated in a series of numerical examples.

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Computational modeling of extreme-loading events
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMPACT SIMULATIONS OF CONVENTIONAL STRENGTH CONCRETE USING EXPLICIT POLYHEDRAL AGGREGATE MORPHOLOGIES

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ABSTRACT

Conventional strength concrete featuring coarse aggregate undergoes complex deformation and damage mechanisms when subjected to dynamic loads. These mechanisms are difficult to capture in a simulation with a homogenous morphology or in a simulation with heterogenous morphology using only elementary geometry. Historically, embedding coarse aggregate or other types of inclusions in laboratory-scale simulations has not been possible due to the resolution of the resulting finite element (FE) meshes. Improvements in computational power coupled with more advanced meshing techniques have made simulating complex morphologies realistic at laboratory scale. This work features simulations that better capture the dynamic solid-state physics of impacts by including polyhedral aggregate shapes within the concrete mesh. These polyhedral aggregate shapes were inscribed within nonintersecting spheres which were generated with ‘ParticlePack’, a piece of software included within the FE software suite ALE3D[1] from Lawrence Livermore National Laboratory. FE meshes were built using a “shape-in” method included in ALE3D. Individual aggregate geometries were stored as ‘STL’ files and imported, or “shaped’, into a homogeneous hexahedral mesh. Impact targets were 16 inches in diameter and 4 inches thick to match physical experiments. Targets were struck with 0.5 inch diameter stainless steel ball bearings over a range of impact velocities. Residual velocities were extracted from simulation data and compared to those from physical experiments for validation. Simulations were also validated visually to compare impact cratering and damage.

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Advanced multiscale and adaptive numerical methods for non-linear solids
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PARALLEL NODE-TO-SURFACE STRATEGY FOR 3D CONTACT MECHANICS PROBLEMS WITH ADAPTIVE MESH REFINEMENT

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ABSTRACT

As contact mechanics problems are locally highly non-linear and non-smooth, their fast and accurate numerical simulation is computationally challenging. Efficient numerical solutions to such problems increasingly rely on high-performance computing (HPC). To optimize the number of degrees of freedom, a relevant mesh discretization is also often sought via adaptive mesh refinement (AMR) strategies. Even so, combining the parallelization of AMR methods with contact mechanics remains a challenging task, current developments on contact numerical solutions focusing either on new non-parallelized adaptive mesh refinement methods or on parallelization ones for uniformly refined meshes.

In previous work, we introduced a generic and parallel node-to-node strategy for solving 3D contact mechanics problems with AMR on hexahedral elements [1]. In this contribution, this strategy is extended to node-to-surface pairing, allowing a wider range of problems to be considered. The main challenge of this extension concerns a mesh partitioning that enables the proposed scalable contact algorithm to be applied effectively. Here, the mesh partitioning is defined via overlapping domain decompositions strategies of the contact interface discretization to guarantee the contact paired nodes to be on the same processes. The contact problem is treated with a penalization technique and is solved thanks to an iterative solver. Once the contact loop converged, the AMR strategy is locally applied and the mesh decomposition is rebalanced with the previously discussed partitioning contact constraints. For the AMR process, a non-conforming h-adaptive mesh refinement solution is considered. This method has already shown high scalability in other contexts [2]. Super-parametric elements are used to preserve the shape of hierarchically refined geometries, even for first-order finite element solutions. In order to carry out simulations, we place ourselves in the MFEM software [2] environment, an open-source finite elements method library. In MFEM, the currently implemented h-adaptive method is enriched with our own estimate-mark-refine approach based on recent works [3].

The proposed AMR-HPC strategy will be confronted with academic and industrial elastostatics test cases.

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Emerging topology and shape optimization techniques in computational design of materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A HYBRID LEVEL-SET/DENSITY TOPOLOGY OPTIMISATION FOR MORPHING STRUCTURES WITH LATTICES AND STRESS CONSTRAINTS IN A LARGE DEFORMATION SETTING WITH MORFEO

Julien Leclerc[*1], Pierre-Alexandre Beaufort[1] and Erin Kuci[1]*

[1]*Cenaero*

ABSTRACT

Coupled to the additive manufacturing, topological optimization helps engineers to imagine efficient and innovative possibilities of design. In particular, it enhances their capacity to create morphing structures and compliant mechanisms.

In this context, this work presents a generic topology optimisation framework applied to morphing structures. This framework is implemented in our in-house finite element software Morfeo. To obtain high performance designs, the optimization relies on several design variables, enabling the introduction of lattices [1]. The topology of the unit cell at the mesoscale is assumed fixed and parametrised by dedicated design variables. It is then represented at the macroscale by an equivalent material behaviour obtained by homogenization.

The optimization problem is modelled thanks to a hybrid method using density-based and level-set XFEM approaches [2]. Thereby, the level-set method enables an accurate surface and stress representation. Moreover, the density-based approach allows holes nucleation during the optimization. Besides, the optimization involves stress constraints under a large deformation setting. Indeed, stress constraints are essential to ensure the mechanical integrity of the designed structure. Moreover, an hyperelastic material model is used to include geometrical non-linearities for more flexibility and better performances in the design.

This framework is applied on morphing wing trailing edges in 2D and other examples in 3D. Taking advantage of the flexibility of our optimization solver, the performances of the resulting structures are compared in terms of model hypotheses and material models (isotropic or lattices).

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Nanomechanics and nanoscale thermal transport for new materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THERMAL CONDUCTIVITY CORRECTION IN W, AND EFFECTS ON DAMAGE CASCADES FROM ATOMISTIC CALCULATIONS

Younggak Shin[1] and Byeongchan Lee[1]*

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ABSTRACT

Atomistic calculations have been widely used to understand the material properties at the nanometer scale, and useful thanks to the all-atom microstructures often in polycrystalline materials. However, the thermal conductivity of a metal predicted from atomistic calculations is typically around 10% of the experimental measurements as only the phonon contribution counts.

In this talk, we introduce an electron-temperature model to be used with interatomic potentials, and show atomistic calculations can still be useful in predicting the thermal conductivity of metals that play a role in fast cooling. As an example, we present irradiation damages in tungsten used as a divertor in fusion reactors, and show how the thermal conductivity correction changes the damage profile.

Our electron-temperature model is an extension to the concept of two-temperature model, and enables both ion-thermal and electron-thermal contributions to the thermal conductivity. The resulting thermal conductivity of tungsten predicted from atomistic calculations is in good agreement with experimental measurements over the wide range of ionic temperature. Here, the energy exchange between ions and electrons is mediated with electron-phonon coupling coefficients, which is made electron-temperature depending in this work. The challenges and the future outlook on electron-temperature models are discussed.

Multiphysics and data-driven modeling for cardiovascular biomedicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BOUNDARY CONDITION FOR THE CEREBROVASCULAR SYSTEM BASED ON SUPPLY AND DEMAND

Chang Min Lee[*1], Seo Yeon Kim[1], Hans Christian Rundfeldt[12], Keun-Hwa Jung[3], Hyeyeon Chang[4] and Hyun Jin Kim[1]*

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ABSTRACT

The demand for improving the precision of medical image-based blood flow simulation has grown significantly over the decades, aiming to diagnose the severity of cardiovascular diseases, predict treatment outcomes, and monitor the cardiovascular system simultaneously. The accuracy of blood flow simulations, however, heavily depends on boundary conditions. Murray’s law or measurement data are conventionally utilized as boundary conditions for the cardiovascular system. Murray's law, however, is known to be highly sensitive to the number and caliber of blood vessels and there is challenge in accurately segmenting small vessels using medical image data. In this study, we develop a physiologic model based on a supply-demand relationship between arteries and tissues and utilize the model as a boundary condition for blood flow simulations of the cerebrovascular system. The geometry of blood vessels and tissues is extracted from MR angiography and T1 MRI, and perfusion territory of each blood vessel and flow rate required for the perfusion territory is estimated using Voronoi tessellation. We validate estimated flows in major arteries against measurements via transcranial color-coded Doppler. Further, we conduct three-dimensional blood flow simulation and cerebral perfusion simulation [1] of healthy and diseased patients using this boundary condition. We compare our results against those obtained using Murray’s law. Additionally, we examine the sensitivity of the proposed boundary condition strategy to the segmented geometry. This study will present a new, robust physiological patient-specific boundary condition strategy for cerebrovascular blood flow simulations.

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A NONOVERLAPPING DOMAIN DECOMPOSITION METHOD FOR EXTREME LEARNING MACHINES SOLVING ELLIPTIC PARTIAL DIFFERENTIAL EQUATIONS

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ABSTRACT

Extreme learning machine (ELM) is a methodology to solve partial differential equations (PDEs) using a single hidden layer feed-forward neural network. It pre-sets the weight/bias coefficients in the hidden layer with random values and fixes them throughout the computation, and uses a linear least squares method for training the parameters of the output layer of the neural network. It has been known much faster than the Physics informed neural networks. However, classical ELM requires to solve a least squares system of large size to get the high level of representation for the solution so that it comes with a computational burden. In this paper, we propose a nonoverlapping domain decomposition method (DDM) for ELMs, that not only reduces the training time of ELMs, but is also suitable for parallel computation. In numerical analysis, DDMs have been widely studied to reduce the time to obtain finite element solutions for elliptic PDEs through parallel computation. Among these approaches, the nonoverlapping DDMs are attracting most attention. Motivated by this method, we introduce local neural networks which are valid only at corresponding subdomains and an auxiliary variable at the interface. Then, we construct a system on the variable and the parameters of local neural networks. A Schur complement system on interface can be derived by eliminating the parameters of the output layer. After that, the auxiliary variable is directly obtained by solving the reduced system and then the parameters for each local neural network are solved in parallel. Numerical results that verify the acceleration performance of the proposed method with respect to the number of subdomains are presented.

Advanced discretization schemes and solution strategies for computational structural dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT OF HIGH-ORDER MULTI-SUB-STEP IMPLICIT TIME INTEGRATION METHODS

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ABSTRACT

This study aims to develop a higher-order implicit multi-sub-step time integration method. The study demonstrates that the proposed s-sub-step schemes, with $2 \leq s \leq 5$, attain (s+1)th-order accuracy while simultaneously ensuring unconditional stability and dissipation control. The proposed composite s-sub-step method does not require acceleration vectors during calculation; instead, these vectors are obtained using finite difference approximation (FDA). We present the outcomes of linear and nonlinear example solutions to validate our theoretical results. These results indicate that the proposed multi-sub-step technique, in comparison to conventional methods, can yield more accurate solutions.

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Microstructures of chemically complex materials and their impacts on material properties from multiscale simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPLORATION OF CHEMICAL SPACE FOR STABLE SOLID-STATE ELECTROLYTES WITH HIGH ION CONDUCTIVITY

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ABSTRACT

Lithium halides Li3MX6 (M = trivalent metals; X = Cl, Br) have emerged as promising solid electrolytes for high-capacity, all-solid-state lithium-ion batteries, acclaimed for their outstanding electrochemical stability and high ionic conductivity. Despite of their potential, the correlation between alloy compositions and resulting material properties has not been fully elucidated. This study aims to bridge this gap by proposing a design strategy for lithium halides, targeting optimized performance in material stability and ion conductivity for advanced high-voltage Li-ion batteries. We systematically investigate crystal structures, phase behavior, electronic properties, and ionic conductivities through extensive density functional theory (DFT) and ab-initio molecular dynamics simulations, incorporated by on-the-fly machine learning energy/atomic force predictions to speed up chemical space exploration. Our analysis indicates significant impacts from varying M:X ratios on structural stability. Mixed halogen anions, Cl and Br, notably alter the material's structure, while different trivalent metal substitutions lead to distorted lattices, affecting Li-ion diffusion activation energy. These findings offer a pathway for the tailored design of lithium halide electrolytes in advanced battery technologies.

Keywords: ab-initio molecular dynamics, ionic conductivity

Data-driven approaches for solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NEURAL OPERATOR ACCELERATED DESIGN OF MULTIFUNCTIONAL METAMATERIALS SUBJECT TO HETEROGENEOUS FIELDS

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ABSTRACT

Data-driven metamaterials design has offered a compelling route to bring the multiscale architectures to their full potential. In doing so, most prior works resorted to the mapping from a parameterized unit cell geometry to the corresponding homogenized properties, such as Young's moduli and transmission spectra. Skipping raw solution fields, any surrogate obtained with this shortcut based modeling features little generality, resuability, and transparency. To this end, we present a data-driven design framework that can accommodate solutions fields heterogeneously distributed across the system, thus at odds with conventional homogenization assumptions. As a key pillar, we capitalize on implicit Fourier neural operator that serves as a field-to-field surrogate of metamaterial systems subject to heterogeneous fields. Equipped with a gradient-based solution procedure, the proposed framework is demonstrated for the inverse problem on light-by-light plasmonic metasurface, whose electric energy distribution above the array is dynamically programmable via modulation of the incident phase distribution. Within the scope of conventional design approaches, the case study presents grand challenges, primarily (1) drastically varying field distributions with heterogeneous local spikes due to plasmonic resonance and (2) the vast design space, formed jointly by quasi-freeform supercells, incident phase distributions that can be modulated, and multiple on-demand functional states subject to a tradeoff. Tackling all the challenges without simplifications, our framework serves as a design automation tool for metamaterials, beyond the scope of the shortcut based modeling.

Contact and interface mechanics: Modeling and computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A FINITE ELEMENT METHODOLOGY FOR FRETTING WEAR ANALYSIS FOR PRESS-FITTED SHAFTS.

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ABSTRACT

Fretting occurs at the ends of the contact surfaces of press-fitted shafts, such as railway axles, which has a detrimental effect on the fatigue life of the railway axles. Accurately predicting the fretting wear and fretting fatigue life of press-fit shafts is important to prevent derailments and establish appropriate maintenance standards. To predict the fatigue life of press-fitted shafts, quantitative prediction of fretting wear is essential. However, much research is still ongoing because there are many influencing factors on fretting wear, such as changes in friction coefficient, the influence of wear particles, and the selection of an appropriate wear model.

In this study, finite element analysis and numerical wear analysis methods were developed for fretting wear analysis of press-fitted shafts. When a bending load was applied to the press-fitted shaft, the contact pressure and microslip were calculated using finite element analysis. Based on the finite element analysis results, a wear analysis method using the influence coefficient and the matrix inversion method was numerically implemented. Using the developed analysis method, representative wear models including Archard's model and the Dissipated Energy model were applied to predict the fretting wear profile of press-fitted shafts. The analytical results were then compared with experimental results to evaluate the effectiveness of the wear model in fretting wear simulation of press-fit shafts.

Mathematics and algorithms for predictive digital twins (DT)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DIGITAL TWIN DEVELOPMENT AND UNCERTAINTY QUANTIFICATION FOR THE GS-EPS BIOMASS PLANT IN SOUTH KOREA

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ABSTRACT

Biomass power plants should become a key component of Korea's domestic energy supply. Advancements in fluidized bed combustion technology used in biomass power plants increase their combustion efficiency while reducing carbon emissions. Determining the design parameters that optimize the efficiency and stability of the combustion process in the presence of significant uncertainties is costly, time-consuming and often only done suboptimally by experienced operational engineers.

In this work, we seek a robust design to improve the fluidized bed combustion efficiency. We develop a digital twin model of the GS-EPS biomass plant in South Korea that includes a reduced-order model and a GPCE-Kriging surrogate model to efficiently represent the combustion process and constraints. We then perform design under uncertainty in a Bayesian framework to find design and process parameters that decrease the combustion variability and increase the combustion efficiency. This method achieves higher combustion efficiency and robustness while requiring training data of less than a hundred combustion simulations.

Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STRUCTURAL ANALYSIS CONSIDERING ANISOTROPIC CHARACTERISTICS OF FDM 3D PRINTED PARTS

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ABSTRACT

Recently, the usability of 3D printing technology is continuously increasing in various industrial fields due to its high degree of freedom of shape and applicability to various materials. Among various 3D printing process, FDM 3D printing method which extrudes and stacks semi-molten filaments has relatively good equipment durability and low product production costs, so various studies on the FDM 3D printing technology have been steadily conducted. However, One of the main disadvantages of the FDM 3D printing method is that unexpected anisotropic material properties can be occured in the manufactured part due to the nozzle path, voids and bonding strength between filaments, even though isotropic filaments is used in the manufacturing process.[1] In particular, when short/continous fiber reinforced composite materials are considered in the FDM printing process, the above mentioned anisotropic characteristics can become more evident in the manufactured part. According to the above background, the AM-Structural Coupled analysis was conducted in this study in order to consider the unexpected anisotropic characteristics in the manufactured part which caused by various 3D printing conditions such as nozzle path, and so on.

To this end, this study attempted to analyze the effect of the nozzle path on the mechanical behavior of the manufactured part through the tensile tests on ASTM D638 standard specimens with various nozzle paths. In addition, analytical anisotropic material properties dependent on the nozzle path are derived by using a reverse engineering, provied by DIGIMAT-MX, that derives mean-field homogenized material properties based on tensile test data. Finally, based on the derived anisotropic marerial properties dependent on the nozzle path, AM-Structural Coupled Analysis was performed by linking Digimat MAP/CAE and commercial FE softwares such as Abaqus and Ansys. The validity of the proposed analysis model was verified through the AM-Structural Coupled analysis of the tensile specimen manufactured by various 3D printing conditions.

In the future, this study plan to conduct a comprehensive comparison and analysis of the anisotropic properties considering porosity and bonding strength.

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Data science and machine learning applications for composite materials and biomedical engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RECENT PROGRESS IN CONDUCTIVE CEMENTITIOUS COMPOSITES FOR EVALUATING VARIOUS DETERIORATION PHENOMENA: AN OVERVIEW

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ABSTRACT

In recent years, studies have focused on the application of conductive cementitious composites, which incorporate electrically conductive fillers into the cementitious matrix, for evaluating various deterioration phenomena [1]. These composites can be utilized to evaluate the deterioration induced by various external environments (e.g., carbonation, freeze-thaw cycles, chloride ion penetration, and sulfate attack) by examining changes in the electrical properties of the composites [2]. Carbon nanotubes (CNTs) are promising electrically conductive fillers owing to their high aspect ratio and outstanding electrical conductivity. Therefore, a small amount of CNTs can establish electrically conductive pathways in conductive cementitious composites [2,3]. Researchers have developed various conductive cementitious composites incorporating CNTs and have reported that the electrical resistance in the composites increases with exposure time to deterioration [2,3]. This paper provides an overview of recent progress in conductive cementitious composites for evaluating various deterioration phenomena, including the authors' initial work on a machine learning approach to evaluating deterioration in the composites incorporating CNTs [4].

Key Words: Conductive cementitious composites, Deterioration, Carbon nanotube

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Advances in damage & fracture modeling of multiphysics materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHASE-FIELD SIMULATION OF THE FRACTURE-HEALING RESPONSE OF A SELF-HEALING CEMENTITIOUS MATERIAL BASED ON MICROBIAL INDUCED CALCIUM CARBONATE PRECIPITATION

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ABSTRACT

Microbial-induced calcium carbonate precipitation (MICCP) is a biochemical process that utilizes the metabolic activities of microorganisms to facilitate the precipitation of calcium carbonate (CaCO3). Recently, research has shown that MICCP has a promising potential to heal concrete cracks. In this paper, we developed a computational uncoupled damage-healing framework to predict the fracture-healing responses of a multifunctional vascular cementitious composite. The proposed framework integrates a mathematical MICCP healing model into a damage model developed using the phase-field method. For the healing model, the chemical and enzyme kinetics of the MICCP reaction pathway based on ureolytic bacteria (i.e., urease-production bacteria) strain were extensively studied. The model considers the bacterial proliferation, the catalyzed ureolysis reaction, the shift of bicarbonate equilibrium due to pH variation, and then output the predicted CaCO3 precipitation quantity during the reaction pathway. On the other hand, the damage model is based on the FEA with phase-field method, which is utilized to simulate the fracture response of a quasi-brittle material. Therefore, a three-stage computational scheme can be established: In stage 1, the fracture and crack propagation in a virgin concrete structure embedded with vascular network is simulated using the phase-field method. The damage variables at the material points of each element are computed. In stage 2, the concrete structure is unloaded. We assume the necessary chemicals and bacteria are transported to the crack sites through the vascular channels and are immediately ready for reaction. The precipitated CaCO3 estimated by the MICCP model can be converted to the healing ratio, hd, of the damaged structure. The damaged part is assumed to be completely healed when hd=1 and not healed at all when hd=0. Therefore, we can update the damage variables at the material points of each element to the phase-field damage model based on the hd value. Finally, in stage 3, the fracture and crack propagation of the healed concrete structure is then simulated again using the phase-field method. In this study, several benchmark simulations were performed to investigate the MICCP quantity with different initial conditions. Various fracture problems were also used to estimate the mechanical response of the damaged concrete structure after healing. We observe that the simulated load-displacement curve of the healed structure shows a recovery in stiffness depending on the MICCP healing ratio. The proposed framework can be applied to various fracture-healing problems of vascular cementitious materials that adopt MICCP as the healing strategy.

Advances in numerical methods for solution of PDEs
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FINITE ELEMENT MODELING OF BRINKMAN EQUATIONS IN POROUS MEDIA

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ABSTRACT

This study explains the intricate dynamics of fluid movement through tiny rock pores, particularly in challenging underground reservoirs with restricted natural flow. The Brinkman equations are crucial for describing flow in porous media. Utilizing the Brinkman equations, we model fluid flow within micro-layered rock structures. To enhance stability, we introduce a mixed formulation involving velocity, pressure, and vorticity, incorporating the rate of deformation tensor. We introduce Galerkin least-square and least-squares finite element methods to address the incompatibility of finite element spaces, treating velocity, pressure, and vorticity as independent variables. Theoretical analysis delves into critical properties such as coercivity and continuity, providing error estimates. Demonstrating robustness in theoretical findings, these methods achieve optimal convergence rates in the L2 norm by incorporating stabilization terms, even with low-order basis functions. Furthermore, we extend these methods to simulate pore-scale flow in porous media, validating their efficacy. Notably, as the inlet velocity increases, there is a significant amplification in the average pressure difference compared to solutions governed by the Stokes equation.

Recent advances on interfaces dynamics modeling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NEURAL NETWORKS WITH LOCAL CONVERGING INPUTS (NNLCI) FOR SOLVING PDES IN VARYING AND MULTI DOMAINS WITH COMPLICATED INTERFACE CONDITIONS

Zhen Chao[1], Harris Cobb[2], Hwi Lee[2], Yingjie Liu[2] and Dexuan Xie[3]*

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ABSTRACT

In the series of works (Haoxiang Huang, Yingjie Liu, Vigor Yang, arXiv:2109.09316 and 2204.10424), NNLCI is introduced to predict discontinuities and smooth parts of solutions of the Euler equations in 1D and 2D accurately. For example, in order to predict the solution of the 1D Euler equations at a space-time location, one can design the output of a neural network to be the solution value at the location. If one tries to design the input as the low-cost numerical solution patch in a local domain of dependence of the location (where the information comes from), can the neural network tell if the input is across a shock or in a smooth region ? The answer is no ! The new approach uses two numerical solutions of a conservation law from a converging sequence, computed from low-cost numerical schemes, and in a local domain of dependence of a space-time location as the input for a neural network to predict its high-fidelity solution at the location. Despite smeared input solutions, the output provides sharp approximations to solutions containing shocks and contact discontinuities. The method reduces the complexity by several orders of magnitude compared to a fine grid numerical simulation, has much lower cost to train, and can be used naturally in varying computational domains through training and prediction because it's a local method. NNLCI can be applied to solving the PnP model which describes the electrochemical dynamics around a protein (Zhen Chao, Harris Cobb, Hwi Lee, Yingjie Liu and Dexuan Xie.) This model involves nonlinear Poisson systems in multiple subdomains connected with complicated interface conditions. We will demonstrate how NNLCI can be used in this problem to reduce the complexity and training costs.

Recent advances in numerical methods for interface problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A SCHUR COMPLEMENT METHOD FOR THE STOKES-BIOT SYSTEM AND ROM IMPLEMENTATION

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ABSTRACT

We present a partitioned method for the Stoke-Biot system based on a monolithic formulation of the problem, which employs a Schur complement equation for a Lagrange multiplier. This algorithm eradicates the need for iterations between the fluid and structure subdomains and instead allows them to be decoupled and solved separately at each time step. The Lagrange multiplier, representing an approximation of the interface flux, serves as a Neumann boundary condition for each sub-problem, allowing for the fluid and structure to be solved independently at each time step. To reduce computational costs, we consider implementing a reduced order model (ROM) for one or both subdomains. The Schur complement method developed for the original Stokes-Biot system can be utilized to couple a reduced order model with either a full order model or a reduced order model on the other subdomain. We show numerical results demonstrating the method's capability to capture each type of coupling.

Multiscale computational and data-driven approach of advanced materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MOLECULAR DYNAMICS STUDY ON ELECTROELASTIC PROPERTIES OF HEXAGONAL BORON NITRIDE NANOSTRUCTURE: COMBINED EFFECT OF VACANCY STRUCTURE AND TEMPERATURE

Jaewon Lee[*1] and Seunghwa Yang*[1]

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ABSTRACT

As the demand for wearable and implantable devices increases, low-dimensional piezoelectric materials have received considerable attention as next-generation nanomaterials. Especially, two-dimensional piezoelectric nanomaterials are promising due to their flexible, atomically thin, and transparent characteristics with a high surface-to-volume ratio compared to three-dimensional piezoelectric crystals. Hexagonal boron nitride nanosheets(BNNS) have been one of the promising piezoelectric low dimensional nanomaterials owing to their ultrahigh mechanical properties, low toxicity, and high chemical/thermal stability, suggesting great potential for energy harvesting devices in biomedical applications.

In order to utilize BNNS in such elaborate fields, it is necessary to fully understand the structure-operation environment-properties relationship. Nevertheless, it was only three to four years ago that the piezoelectric coefficient of mono-layer hexagonal boron nitride was first measured experimentally, and most of the piezoelectric properties were theoretically predicted based on the first principle calculation. Therefore, there exists a technological gap between actual application and theoretical prediction. Although several researchers have predicted the piezoelectric properties of BNNS through molecular dynamics simulation to bridge this gap, an integrated analysis of the structure-temperature-properties relations for electoelastic properties of BNNS has rarely been studied yet.

In this study, molecular dynamics simulation was conducted to investigate the effect of vacancy defect and temperature on the electroelastic properties of BNNS, each of which is representative of structural defects and service conditions in nanomaterials, respectively. Based on the direct piezoelastic Maxwell relations, the strain-stress relation and strain-electric displacement relationships of BNNS were predicted by applying linear elastic strain along the armchair direction. To describe the electroelastic behavior, the Tersoff potential and rigid ion approximation were adopted. As a result, the vacancy defects and temperature showed a non-negligible influence on the piezoelectric constant of BNNS. The vacancy defect either increases or decreases the piezoelectric constant of BNNS depending on the alignment of BN di-vacancy, while Young’s moduli were always degraded by the vacancy. Furthermore, such an abnormal increase of piezoelectric constant with di-vacancy was more clearly observed at lower temperature conditions. To analyze the mechanism of these phenomena, the atomic displacement of B and N around the defects was monitored and compared by vacancy type and temperature based on the linear piezoelectricity theory. Finally, the possibility of defect engineering by controlling the vacancy defects in BNNS with controlled service temperature conditions was discussed.

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Data science and machine learning applications for composite materials and biomedical engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NEW ELASTODYNAMIC HOMOGENIZATION THEORY OF FINITE-SIZE APERIODIC MEDIA AND ITS MACHINE LEARNING-BASED IMPLEMENTATION

Jeong-Ho Lee[1] and Grace Gu*[1]

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ABSTRACT

Architected materials, such as composites and metamaterials, have been extensively utilized across academia and industries for their tunable, superior functionalities, e.g., high stiffness with lightweight. Their design is based on engineered microstructure patterns and/or heterogeneous material distribution rather than synthesizing chemically new materials, from which they can exhibit unprecedented features in the overall behavior at the macroscale even though they are, at the microscale, composed of typical materials in nature. Homogenization theories have been widely employed to evaluate the functionality of architected materials by seeking to define the effective material properties of an equivalent homogeneous media. This approach can simplify the analysis of architected materials by making understanding the fundamental physics behind their macroscopic behavior easier. For instance, elastodynamic homogenization on architected materials with asymmetric microstructures gives a non-classical coupling property, called Willis coupling, between stress and velocity, which plays a role in understanding and predicting a more accurate representation of wave propagation. However, most of the developed homogenization theories have limitations that challenge their application for general finite-size aperiodic media. First, they assume a volume average or asymptotic expansion for the bridge between microscopic and macroscopic fields, which only works for limited circumstances, such as when microstructures are at the subwavelength scale or have a much smaller scale than the macroscale of interest, respectively. Second, they only consider a partial domain of the target medium to be homogenized since they rely on representative volume elements and assume periodic boundary conditions. That is, it is not possible in general cases to consider the exact design and geometry of the target medium. These limitations not only hinder the accurate prediction of effective material properties but also, when it comes to practical applications such as finding optimal designs for a target effective property, restrict the design space of architected materials to periodic designs. Therefore, to overcome the limitations, we formulate a new elastodynamic homogenization theory via a polarization approach using infinite-body Green’s function of a comparison homogeneous medium. As this theory builds on Green’s function, the resultant homogenization equation inherently includes integral operators that lead to high computational costs. We resolve this issue by developing a deep neural network, in which the homogenization equation is used as a physics-informed loss, and apply this developed network to an example problem for homogenization-based design optimization.

Recent advances in discretization techniques for coupled problems in incompressible fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HYBRIDIZABLE DISCONTINUOUS GALERKIN METHODS FOR COUPLED SYSTEMS OF POROELASTICITY AND FREE FLOW EQUATIONS

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ABSTRACT

In this work we develop and analyze hybridizable discontinuous Galerkin (HDG) methods for problems such that the Stokes and Navier-Stokes equations and the Biot consolidation equations are coupled with interface. In our HDG methods the compressibilities of fluid and poroelastic matrix, and the fluid mass in poroelastic domain are strongly conservative.

EFFICIENT ESTIMATION OF HIGHWAY BRIDGE SEISMIC RESPONSE USING PROBABILISTIC LEARNING ON MANIFOLDS (PLOM)

Jeonghyun Lee[1], Kuanshi Zhong[2], Sanjay Govindjee[3] and Gregory Deierlein[1]*

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[3]*University of California, Berkeley*

ABSTRACT

Seismic risk analysis of distributed bridge networks is a crucial component of evaluating the disruption to transportation systems and the resultant travel time increase following earthquakes. The core idea behind such analyses is to assess the behavior of individual bridges at each discrete location and propagate the results throughout an entire portfolio to gain a holistic understanding of the regional impacts. The key limits in this process are obtaining high-resolution estimates of individual bridge responses through nonlinear analysis (quality) and the inherent need to repeat this procedure given a large inventory (quantity). We propose a surrogate modeling approach to efficiently assess the earthquake response of bridges while attaining both goals using Probabilistic Learning on Mainfolds (PLoM). PLoM is particularly suited to the problem given its multidimensional nature where we need to consider both the variability in the bridge design parameters and the site-specific characteristics.

Our approach predicts both the ultimate capacity of a bridge as well as the dynamic response of the bridge leading up to collapse. For both applications, the surrogate model is developed on a training set of bridges sampled from a large design space that are subjected to a grid of ground motions. The surrogate model's performance is tested on an archetype bridge at 16 real-world locations. We also provide a streamlined approach to tune the two PLoM modeling parameters (i.e., diffusion-maps kernel size and number of diffusion-map components) applicable to various sites and bridge designs, thereby reducing the burden on the end-user. The final model allows users to evaluate various damage characteristics (e.g., rebar fracture) of bridges at multiple sites and intensity levels. Such models will not only enable high-resolution regional studies, but also the evaluation of performance under preventative scenarios (e.g., which types of retrofits are most beneficial, which set of bridges should be prioritized?). Lastly, comparisons of the proposed surrogate model's computational efficiency to conventional approaches along with further enhancements to its efficiency are discussed.

Advance and application of meshfree methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATION OF BOUNDARY INTEGRAL QUADRATURE METHOD TO A CIRCULAR TORSION BAR WITH AN EDGE CRACK

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ABSTRACT

Regarding the torsion problem of elastic cylindrical bar with an edge crack, the boundary integral quadrature method (BIQM) in conjunction with the dual formula is employed to solve the stress function. Comparing with the conventional dual boundary element method (BEM), the present method is free of mesh generation. To achieve this benefit, the adaptive exact solution, parametric representation and Gaussian quadrature play important roles. By introducing the adaptive exact solution, the singular integral in the sense of the Cauchy principal value can be skillfully determined. For the collocation point located on the ordinary boundary, we adopt the original adaptive exact solution. For the collocation point located on the crack, the adaptive exact solution is rederived by using the harmonic basis of elliptical coordinates. To realize the effect upon the elastic cylinder due to the crack, the torsional rigidity and the stress intensity factor (SIF) are considered to calculate. To conveniently determine the torsional rigidity, the domain integral formula is transformed into the form of the boundary integral. The computation of the SIF is dependent on the unknown boundary density near the crack tip. Therefore, the extra computation of the two shear stress fields is free. It is interesting that the self-regularized approach can be also employed to obtain the correct unknown boundary density without using the dual formula in the present method. To check the validity of above two manners, the conventional dual BEM is also adopted to examine those results. Finally, two elastic cylindrical bars containing different edge cracks are considered. One is a radial edge crack and the other is a slant edge crack.

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Multiscale computational and data-driven approach of advanced materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE APPROACH TO EVALUATE FRACTURE TOUGHNESS OF POLYMER NANOCOMPOSITES BY CONSIDERING COHESIVE FAILURE MODE

Jihun Lee[1], Haolin Wang[1], Jae Hun Kim[1] and Hyunseong Shin[1]*

[1]*Inha University*

ABSTRACT

The covalent grafting between the nanofillers and the polymer matrix is regarded as a useful design factor to tailor the mechanical properties. Polymer nanocomposites including covalent grafting form a strong interphase due to strong interfacial interactions between nanofillers and polymer matrix. Furthermore, these strong interfacial interactions can lead to cohesive failure mode in the debonding mechanisms [1]. However, since the conventional multiscale fracture toughness model [2, 3] did not account for the cohesive failure mode, it is necessary to develop a theoretical model evaluating the fracture toughness of polymer nanocomposites by considering the cohesive failure mode. In this paper, we develop a multiscale fracture toughness model reflecting the cohesive failure mode in the debonding mechanisms. The multiscale strategy was modified by incorporating the microscopic damage mechanisms (cohesive failure mode in the debonding mechanisms and plastic yielding of nanovoids), which occur near the macroscopic crack tip. The influence of microscopic energy dissipation on the strain energy release rate of nanocomposites according to grafting ratios was quantitatively evaluated using the developed multiscale model. In addition, to investigate the effect of grafting ratios on surface roughness, the assessment of surface roughness related to fracture resistance was performed. This assessment was calculated via remaining atoms on the nanofiller surface using traction–separation behavior in molecular dynamics simulations. When collecting the results of surface roughness with those of fracture toughness obtained from the proposed multiscale fracture toughness model, it implies that excessive amount of covalent grafting may not contribute to the fracture toughness improvement of polymer nanocomposites. In conclusion, the proposed multiscale model is expected that the proposed multiscale model can be used as a design guideline for improving the fracture toughness of polymer nanocomposites.

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Trustworthy multi-fidelity and data-driven models for computational applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A STUDY ON MULTI-FIDELITY SURROGATE FOR MULTIPLE LOW-FIDELITY INFORMATION

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ABSTRACT

Over the past few decades, surrogate models (also known as metamodels) have been widely employed in optimization based on costly computer simulations to enhance computational efficiency. However, even with advancements in computing performances, obtaining sufficient data remains challenging when simulation times are prohibitively high. To alleviate these difficulties, various techniques such as screening, mapping, decomposition, and auxiliary information have been developed. Particularly, leveraging low-fidelity data as auxiliary information is considered a promising approach. Multi-fidelity (MF) surrogate models, which combine high-fidelity samples with low-fidelity samples, have proven effective in addressing this issue across various real-world problems [1]. Nevertheless, in practical scenarios, the quality of low-fidelity data may not always be good [2], and dealing with diverse types of low-fidelity data from multiple sources adds complexity [3].

As a solution to these challenges, this study proposes a MF methodology for utilizing low-fidelity information from multiple sources. The proposed approach addresses the creation of MF surrogate models from the perspective of low-fidelity data and is developed based on cross-validation error. Additionally, the proposed method uses the well-known Kriging-based MF surrogate. Numerical test results demonstrate the superior performances of the proposed approach compared to the existing methods.

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Fracture, damage and failure mechanics of cementitious materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BLAST ANALYSIS OF HIGH-PERFORMANCE FIBER-REINFORCED CEMENT COMPOSITE PANELS

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ABSTRACT

This paper numerically investigates the performance of RC and high performance fiber-reinforced cement composite (HPFRCC) panels suffered from near field TNT explosion using MM-ALE method. HPFRCC, which is one of advanced construction materials, is promising for application to protective structures [1]. A Karagoziam & Case (K&C) model [2], which is one of plastic-based concrete material models, can describe accurately the response of concrete structures subjected to blast and impact loadings. However, since automatically determined parameters are based on plain concrete, these are not appropriate for HPFRCC. The K&C model is calibrated based on the quasi-static and dynamic experimental data of HPFRCC. The modified K&C model is implemented into LS-DYNA [3] program to perform numerical simulations of the HPFRCC panels. The accuracy and reliability of the numerical simulations using MM-ALE method were verified through comparison with the LBE method and test results. The HPFRCC panel has superior blast resistance performance than normal concrete from simulations and experiments. Additionally, parametric studies are conducted to investigate the differences between the explosive characteristics and failure shape of the specimens according to the modelling shapes of TNT explosive and scaled distance.

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EARLY DETECTION OF SURGE PHENOMENA IN AIR CONDITIONING SYSTEMS THROUGH SYNTHETIC DATA GENERATION

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ABSTRACT

Air as a refrigerant in compressors provides an environmentally sustainable option that significantly lowers the global warming potential associated with traditional refrigerants. However, it directly leads to challenges in maintaining the compressor system's reliability and efficiency. Moreover, the necessity to operate the compressor's rotor system at high speeds for air refrigeration increases the risk of surge phenomena, directly threatening the compressor's integrity and operational safety. The study employs a data-driven approach, using machine learning to detect surge events in advance. However, replicating transient phenomena such as surge events in a testbed is not only difficult due to the complexity of artificially creating these conditions, but it also poses significant risks to both humans and mechanical systems, thereby complicating the process of data acquisition. To address the issue of data scarcity, this study generated synthetic data distributions that share similar characteristics with real data, utilizing machine learning techniques. Specifically, the research focused on ensuring that the datasets, inherently time-series in nature, were developed while preserving the patterns and dynamic characteristics inherent to their temporal progression. The methodologies proposed offer solutions to the challenges posed by air refrigerants and are applicable to other engineering fields facing data limitations.

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Current trends in phase-field modeling and computations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A PHASE-FIELD DESCRIPTION OF THERMO-HYDRO-MECHANICAL PROPAGATING FRACTURES

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[3]*The University of Texas at Austin*

ABSTRACT

This study introduces a thermo-hydraulic-mechanical (THM) model for fracture propagation using a phase-field approach. We developed a computational framework incorporating rigorous and efficient iterative coupling, high-fidelity physics-preserving finite element methods, and adaptive mesh refinement. In our governing system, we focus on four solution variables: displacements, phase-field, pressure, and temperature. These variables are determined through a vector-valued mechanics problem, a phase-field variational inequality, and scalar-valued pressure and temperature problems, respectively. The resulting overall problem forms a coupled variational inequality system. Our solution algorithm builds upon the well-known fixed-stress algorithm, solving displacements-phase-field, pressures, and temperatures sequentially. The displacements-phase-field component is addressed in a quasi-monolithic fashion. To ensure local mass conservation, we utilize enriched Galerkin finite elements for the pressure equation, and similarly for the temperature equation. Local mesh adaptivity enables the use of small phase-field length-scale parameters, ensuring numerical accuracy while maintaining reasonable computational costs. We validate our new model and algorithmic developments through numerical tests.

Physics-informed machine learning for numerical modelling in engineering and science
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STUDY ON ACTION-BASED PINN TO PREDICT THE BEHAVIOR OF THE SYSTEM HAVING PHASE TRANSITION

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ABSTRACT

Liquid crystals can be controlled by external stimuli, exhibiting both crystalline and fluidity. Due to these distinctive mechanical properties, liquid crystals have garnered lots of interest. With this interest, several numerical models describing the behavior of the liquid crystal have been presented. The Landau-de Gennes free energy model is one of the most representative models to be used for describing the phase of the liquid crystal. Several approaches to simulate the relaxed state of the liquid crystal have been successfully proposed by searching the minimum point of the Landau-de Gennes free energy. However, the multi-well potential of this free energy is a critical obstacle to finding the minimum point by solving the Euler-Lagrange equation of Landau-de Gennes free energy. Consequently, the simulations to predict the equilibrium state of the liquid crystal system based on the Landau-de Gennes free energy model perform gradient-based minimization. Since gradient-based minimization requires iterative computation, these simulations encounter the challenge of acquiring high-fidelity results.

To ease the issue, we leverage the reusability of the neural network through transfer learning. Transfer learning needs much less training time by updating only a few deep layers of the pre-trained neural network. Among the neural networks, we applied this advantage to the PINN (Physics-informed neural network) to analyze the liquid crystal system. The PINNis an emerging neural network embedding the physical information of the system in the form of partial differential equations. The PINN has drawn a lot of attention in various physical domains with showing successful solving several physical problems[1]. In this study, we propose a modified version of PINN, the Action-based PINN, minimizing the action functional to predict the equilibrium state of the liquid crystal system. By the gradient-based minimum point searching, the Action-based PINN successfully predicts the ground state of the system having phase transition.

The accuracy and effects of the proposed network in this study are demonstrated by comparing the prediction results of the Action-based PINN with those of standard PINN in several numerical examples. Additionally, our study delves into the advantages of the Action-Based PINN, especially its enhanced reusability, offering a significant improvement over traditional numerical methods.

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Scientific deep learning
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN ENERGY-BASED ADVERSARIAL FORMULATION OF PHYSICS-INFORMED NEURAL NETWORKS FOR SADDLE POINT PROBLEMS INVOLVING DIELECTRIC ELASTOMERS

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ABSTRACT

Keywords: Physics-informed neural networks, Deep energy method, Saddle point problem, Adversarial networks, Dielectric elastomers

Multiphysics systems, where two or more physical phenomena are coupled, play a crucial role in various fields including biophysics, geophysics, and aerospace engineering. These complex systems are modeled using multiple partial differential equations (PDEs) with coupling terms, posing substantial challenges in mathematical formulation, numerical analysis, algorithm design, and software engineering. Addressing these challenges, recent machine learning advancements, specifically physics-informed neural networks (PINN), have enabled more unified and flexible solutions to a broad range of PDE problems [1]. The deep energy method (DEM), a variant of PINN, utilizes neural networks to efficiently tackle PDEs by minimizing associated functionals [2]. However, its application has been mainly limited to scenarios with simpler variational principles. In contrast, multiphysics systems often present intricate saddle point problems involving multiple field variables.
To effectively address this complexity, we propose an adversarial deep energy method (adversarial DEM) that employs multiple neural networks in an adversarial relation. Adversarial DEM is particularly tailored to tackle the minimax variational principle through saddle point optimization algorithms, largely expanding the applicable range of the existing DEM. Our method has been applied to electromechanical coupling in dielectric elastomers, serving as a concrete example of a multiphysics system with the minimax variational principle. The results from benchmarking problems in dielectric elastomers showcase the strength in handling diverse material models and accurately capturing intricate nonlinear phenomena like buckling in electromechanical coupling. In summary, our method addresses the existing limitations of conventional approaches in modeling multiphysics systems, paving way for the application of machine learning in complex system simulations.

Acknowledgements
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Design beyond optimization: Why, what if, and how much?
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NEW ADAPTIVE KRIGING-BASED OPTIMIZATION (AKBO) FRAMEWORK COMBINING A TRUNCATED CONSTRAINT FUNCTION (TCF) METHOD AND A NEAR CONSTRAINT BOUNDARY SEARCH (NCBS) ALGORITHM

Ungki Lee[*1]*

[1]*Korea University Sejong Campus*

ABSTRACT

Adaptive Kriging-based optimization (AKBO) efficiently performs optimization by employing adaptive sampling methods that sequentially update Kriging model [1]. To solve constrained optimization problems, existing adaptive sampling methods add samples based on probability of feasibility (PoF) representing the probability that all constraints are satisfied [2]. However, these methods have the limitation that samples are added inefficiently when the PoF is inaccurate. Therefore, this study proposes a new AKBO framework that is robust to instability of PoF in adaptive sampling. To this end, a near constraint boundary region that is expected to be close to the constraint boundary is defined based on a probability measure. Then, a near constraint boundary search (NCBS) algorithm, which explores the sample point that minimizes the objective function within the near constraint boundary region, is developed for global search, whereas a near optimum search (NOS) algorithm, which searches for better solutions that may exist near the current optimum candidate, is developed for local search. To alleviate the distortions of the Kriging model that may occur due to the highly nonlinear response, a truncated constraint function (TCF) method that limits the extremely violated constraint values used in the design of experiment (DoE) of the Kriging model is also proposed. This study verifies the performance of the proposed AKBO framework through the shared autonomous electric vehicle (SAEV) system design optimization problem. Comparison of optimum designs derived from various optimization methods shows that the proposed AKBO framework derives the feasible global optimum with high accuracy and efficiency.

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Multiscale computational and data-driven approach of advanced materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TEMPORAL HOMOGENIZATION METHOD FOR VISCOELASTIC–VISCOPLASTIC MATERIALS SUBJECTED TO CYCLIC LOADING

Wonjoo Lee[1] and Hyunseong Shin*[1]

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ABSTRACT

In this study, a formulation for temporal homogenization was developed for application to the viscoelastic-viscoplastic model. Two types of temporal homogenizations were explored: non-updated temporal homogenization and updated temporal homogenization. The non-updated temporal homogenization employs a constitutive equation with higher-order differential forms in the viscoelastic-viscoplastic model. On the other hand, the updated temporal homogenization involves separating the local initial boundary problem by applying a constitutive equation with higher-order differential forms in the viscoelastic-viscoplastic model. The solutions obtained (i.e., local displacement, strain, and stress fields) for the local initial boundary problem are also utilized for the global initial boundary value problem. Volterra equations or Laplace transforms are not required to solve the local initial boundary problem. The novelty of this study lies in the efficient formulation of temporal homogenization for viscoelastic-viscoplastic materials. Notably, this is the first attempt to develop an updated temporal homogenization formulation for viscoelastic-viscoplastic materials without relying on Volterra integrals to solve the local initial boundary problem.
In conclusion, the initial boundary value problems are divided into macro-, micro-chronological terms. To validate this approach, two examples were considered: (i) uniaxial cyclic loading on a one-dimensional bar, (ii) multiaxial cyclic loading on a three-dimensional bar. By comparing the accuracies of non-updated and updated temporal homogenization formulations, it becomes evident that the updated temporal homogenization formulation yields more accurate results. The first advantage is that stress updates are not used in solving the local initial boundary value problem. The second advantage, as demonstrated by the verification examples, is that the local initial boundary value problem subjected to local cyclic loading on the viscoelastic-viscoplastic model was resolved with high accuracy.

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DATA ASSIMILATION THROUGH SEMI-GAUSSIAN BAYESIAN UPDATE

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ABSTRACT

This study proposes a semi-Gaussian Bayesian update framework for optimal control and data assimilation. In particular, the study focuses on an ensemble-based approach for such goals. The framework will provide insights into the meaning of inflation and sampling error correction (or localization) commonly used in the ensemble-based Bayesian update methods, such as ensemble transform or adjustment Kalman filters. The study further provides a strategy for designing a new sampling error correction for error correction instead of the distance-based ad hoc approach.

Verification techniques in computational physics and applied mathematics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VERIFICATION METHODS FOR OBLIQUE SHOCK REFLECTIONS

Allyson Leffler[1], Jasper Thrussell[1], Steven Anderson[1] and Jim Ferguson[1]*

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ABSTRACT

Oblique shock reflections occur in a variety of instances where a supersonic flow is concavely deflected by a contact surface. One such instance of this flow phenomenon is when a planar shock impinges on a wedge. These shock reflections can vary drastically in complexity depending on the initial Mach number of the planar shock, the number of facets on the wedge, and their corresponding angles. As multiple wedges are stacked on top of one another, the interactions between the reflected shocks become increasingly complex and difficult to analyze. This type of wedge configuration is commonly found in a variety of engineering applications and shock experiments and can be thought of as the discretization of a curved geometry. Due to the widespread use of computational fluid dynamics, understanding the level of confidence associated with numerical simulations of this flow phenomenon is necessary.

Ideally, analytical solutions could be used to draw conclusions about how well a simulation produces an expected behavior, but for this type of flow phenomenon, limited analytical solutions exist. Thus, it is necessary to explore and develop novel verification techniques. We present various assessments of numerical simulations of a planar shock impinging on both single faceted and double faceted wedges. This study proposes and demonstrates the utility of using method of characteristics to obtain semi-analytical solutions for various oblique shock reflections. These solutions can then be used as a verification tool to draw quantitative comparisons and establish confidence in the simulations.

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MODELING IMMERSED GRANULAR FLOWS

Vincent Legat[*1], Nathan Coppin[1], Michel Henry[1], Simon Yans[1] and Jonathan Lambrechts[1]*

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ABSTRACT

An unresolved Computational Fluid Dynamic-Discrete Element Method (CFD-DEM) model for the simulation of flows mixing fluid and grains is presented. The grains trajectories are solved at a fine scale using a discrete element method. It provides the velocities and the trajectories of the grains with an accuracy that is needed to describe microscopic phenomena like clogging in pipe happening in these flows. Solved at a coarse scale using the finite element method, the fluid motion is deduced from a mean continuous representation of the fluid phase giving computational performance and keeping variables evolutions that are of interest for a lot of simulation processes.

The collapse dynamics and runout of columns of elongated grains are numerically are investigated in dry and immersed conditions. The elongated grains are modelled as rigid aggregates of disks. The column aspect ratio is systematically varied from 0.125 to 16 in order to span short and tall columns. To analyse the effect of the initial grain orientation, columns with an initial grain orientation that is either random or aligned with a given direction are both considered. Collapse dynamics, both in dry and immersed cases, exhibit a power law dependency for the runout as a function of the column aspect ratio. The effect of the fluid mainly results in a decrease of the runout distance. Interestingly, the collapse dynamics and runout are not significantly affected by the initial orientation of the grains, except maybe in the extreme case where the grains are all horizontally oriented, which geometrically prevents the collapse.

https://www.migflow.be/

N. Coppin, H. Michel, M. Cabrera, E. Azéma, F. Dubois, V. Legat, J. Lambrechts
Collapse dynamics of two-dimensional dry and immersed granular columns of elongated grains
Physical Review Fluids, Vol 8. 9:094303 (2023)

M. Constant, F. Dubois, J. Lambrechts, V. Legat
Implementation of an unresolved stabilised FEM-DEM model to solve immersed granular flows
Computational Particle Mechanics, Vol. 6, 213-226 (2019)

Advanced numerical methods for the modeling and optimization of coupled dynamical systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STRUCTURAL REINFORCEMENT AND VIBRATION REDUCTION WITH ELASTIC AND VISCOELASTIC MATERIALS USING TOPOLOGY OPTIMIZATION

Antoine Legay[*1] and Sylvain Burri*[1]

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ABSTRACT

This work addresses mechanical design problems such as structural reinforcement adding elastic material or vibration reduction using viscoelastic layers.
The aim is thus to attach on a pre-existing given structure a design domain in order to improve the behavior of this elastic structure, according to an objective function.
This can be useful when one wants to use, for example, additive manufacturing to reinforce a pre-existing structure or to maximize structural damping using viscoelastic layers.
Two objective functions are tested in both linear statics and dynamics: a compliance based objective function and a displacement based one.
The topology optimization formulation based on the Solid Isotropic Material with Penalization (SIMP) method is then used to minimize the objective function. It is solved by the Modified Optimality Criteria (MOC) algorithm.
In the dynamic case, written in the frequency domain, the two proposed objective functions include the viscoelastic material model (a Zener fractional derivative one) used to fill the design domain.
The displacement criteria is developed using a general formula able to take into account as many as degree of freedom as necessary.
Finally, some applications based on beams and CubeSat-like structures are shown in this article.
The proposed examples show that in both statics and dynamics, the optimization of a restrained design domain attached to an existing structure can improve its behavior: stiffness improvement or vibration reduction.

Certification of simulations and model adaptation in computational science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A POSTERIORI ERROR ESTIMATORS AND MODEL REDUCTION FOR MULTISCALE PROBLEMS

Frederic Legoll[*1], Ludovic Chamoin[2], Arthur Lebee[3] and Jean Ruel[3]*

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[3]*École des ponts ParisTech*

ABSTRACT

This talk is devoted to the numerical simulation of multiscale problems. The multiscale nature may stem from the presence of a heterogeneous microstructure, as for instance in composite materials. It may also stem from the geometry of the domain. A typical example is the case of elongated structures, such as plates, where the thickness of the structure is much smaller in one direction than in the others.

Dedicated numerical methods have been proposed in the literature for each of these cases. For composite materials, a possibility is to resort to the Multiscale Finite Element Method (MsFEM), a Finite Element type approach where the basis functions used to generate the approximation space are precomputed and are specifically adapted to the problem at hand. For plates, finite element methods typically distinguish the in-plane directions from the thickness direction. PGD-type approaches are also a method of choice, again to handle differently the various directions.

In this context, we will describe efficient tools enabling to certify the numerical simulations, with respect to both discretization and model errors.

This talk is based on joint works with L. Chamoin, A. Lebee and J. Ruel.

Related reference: L. Chamoin and F. Legoll, An introductory review on a posteriori error estimation in Finite Element computations, SIAM Review, vol. 65 (4), 963-1028 (2023).

UNCERTAINTY QUANTIFICATION IN 3D PHYSICS-BASED SIMULATIONS WITH A NEURAL OPERATOR SURROGATE MODEL

Fanny Lehmann[*12], Filippo Gatti[1], Michaël Bertin[2] and Didier Clouteau[1]*

[1]Université Paris-Saclay

[2]Commissariat à l'Energie Atomique et aux Energies Alternatives (CEA)

ABSTRACT

Wave propagation simulations are the core of numerous applications, and they have reached a high level of fidelity thanks to continuous improvements in numerical modelling and computational resources. Physics-based simulations rely on parameters describing the properties of the propagation domain. When simulating wave propagation in the Earth's crust, those properties are subject to large epistemic uncertainties due to the difficulty of conducting geophysical measurements. However, the computational costs of high-fidelity simulations in three-dimensional (3D) heterogeneous domains prevent uncertainty quantification (UQ) via a Monte Carlo-like approach. This work demonstrates using a physics-based deep learning surrogate model to quantify uncertainties in elastic wave propagation.

The surrogate model is based on a Multiple Input Fourier Neural Operator (MIFNO), our extension of the popular Fourier Neural Operator. Fourier Neural Operators rely on the Fast Fourier Transform to learn the frequency representation of Partial Differential Equations (PDEs). Our MIFNO predicts the solution of the 3D elastic wave equation from the properties of the propagation domain and the initial condition. Its main specificities are:
- a factorized architecture that limits the number of parameters and improves the scalability
- a depth-to-time conversion to predict 3D time-dependent variables without a 4D surrogate
- an implementation depending on the input representation (structured grids and vectors)

Training data are obtained from 30,000 High-Performance Computing (HPC) simulations. Each simulation represents the propagation of elastic waves from a random source inside a random 3D heterogeneous domain. Heterogeneities describe the epistemic uncertainties on the properties of the Earth's crust in different regions.

We show that the MIFNO achieves state-of-the-art accuracy when the source is fixed and maintains this accuracy for sources with varying locations and characteristics. It is the first surrogate model with the flexibility of a physics-based solver. Although the high-frequency accuracy is limited by the well-known spectral bias, the MIFNO can still be used for uncertainty analyses on low- and medium-frequency quantities of interest.

For UQ analyses, we focus on the propagation of seismic waves in a region with considerable industrial interests. We sample 500 propagation domains from the distribution of geological heterogeneities and fine-tune the MIFNO on these samples. Based on the current knowledge, all domains are equally likely but earthquakes would have dramatically different consequences in each domain. Thanks to the MIFNO, we predict the ground motion intensity probability distributions that were unachievable with conventional methods.

UQ-TTA student paper competition in uncertainty quantification
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

UNCERTAINTY QUANTIFICATION IN 3D PHYSICS-BASED SIMULATIONS WITH A NEURAL OPERATOR SURROGATE MODEL

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ABSTRACT

Wave propagation simulations are the core of numerous applications, and they have reached a high level of fidelity thanks to continuous improvements in numerical modelling and computational resources. Physics-based simulations rely on parameters describing the properties of the propagation domain. When simulating wave propagation in the Earth's crust, those properties are subject to large epistemic uncertainties due to the difficulty of conducting geophysical measurements. However, the computational costs of high-fidelity simulations in three-dimensional (3D) heterogeneous domains prevent uncertainty quantification (UQ) via a Monte Carlo-like approach. This work demonstrates using a physics-based deep learning surrogate model to quantify uncertainties in elastic wave propagation.

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Training data are obtained from 30,000 High-Performance Computing (HPC) simulations. Each simulation represents the propagation of elastic waves from a random source inside a random 3D heterogeneous domain. Heterogeneities describe the epistemic uncertainties on the properties of the Earth's crust in different regions.

We show that the MIFNO achieves state-of-the-art accuracy when the source is fixed and maintains this accuracy for sources with varying locations and characteristics. It is the first surrogate model with the flexibility of a physics-based solver. Although the high-frequency accuracy is limited by the well-known spectral bias, the MIFNO can still be used for uncertainty analyses on low- and medium-frequency quantities of interest.

For UQ analyses, we focus on the propagation of seismic waves in a region with considerable industrial interests. We sample 500 propagation domains from the distribution of geological heterogeneities and fine-tune the MIFNO on these samples. Based on the current knowledge, all domains are equally likely but earthquakes would have dramatically different consequences in each domain. Thanks to the MIFNO, we

predict the ground motion intensity probability distributions that were unachievable with conventional methods.

Numerical methods, mathematical modeling and analysis in material science
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CONSENSUS-BASED CONSTRUCTION OF HIGH-DIMENSIONAL FREE ENERGY SURFACE

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ABSTRACT

One essential problem in quantifying the collective behaviors of molecular systems lies in the accurate construction of free energy surfaces (FESs). The main challenges arise from the prevalence of energy barriers and the high dimensionality. Existing approaches are often based on sophisticated enhanced sampling methods to establish efficient exploration of the full-phase space. On the other hand, the collection of optimal sample points for the numerical approximation of FESs remains largely under-explored, where the discretization error could become dominant for systems with a large number of collective variables (CVs). We propose a consensus sampling-based approach by reformulating the construction as a minimax problem which simultaneously optimizes the function representation and the training set. In particular, the maximization step establishes a stochastic interacting particle system to achieve the adaptive sampling of the max-residue regime by modulating the exploitation of the Laplace approximation of the current loss function and the exploration of the uncharted phase space; the minimization step updates the FES approximation with the new training set. By iteratively solving the minimax problem, the present method essentially achieves an adversarial learning of the FESs with unified tasks for both phase space exploration and posterior error enhanced sampling. We demonstrate the method by constructing the FESs of molecular systems with a number of CVs up to 30.

Computational fluid dynamics (CFD) and fluid-structure interaction (CFSI): Methods and Applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AERODYNAMICS ANALYSIS OF DRAGONFLY FLAPPING WINGS BASED ON FORCE ELEMENT THEORY

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ABSTRACT

In bionics, the flight patterns and aerodynamics of birds and insects have always been the research topics for humans to discuss aerial flight. Compared with other birds and insects, dragonflies have higher mobility and can hover, make sharp turns, reverse, and have a 360-degree flight.The flight speed of dragonflies is very fast, especially, some species can reach a speed of about 50 kilometers per hour. Therefore, several studies have directed efforts toward the aerodynamics of dragonfly flapping wings, numerically or experimentally. However, for the problem of unsteady flow formed by birds and insects flapping their wings, the commonly used surface pressure integration method to calculate the overall force cannot fully explain the force mechanism between the flow field and the force exerted on the body. To date, there have been many researches discussing the flight mode of dragonflies, but no matter whether it is numerical simulation, bionic mechanism design, or exploring the real dragonfly, it is lacking to clearly describe how the vorticity has the lift-drag effect on flight. In the present work, by applying the Force Element Theory, the vorticity was linked with the force and the flow field obtained by applying the CFD, and the sources of force in dragonfly in-phase stroking and counter stroking, as well as the changes of each force element term in a period were discussed.The main findings include: (i) In-phase stroking flight is the way the dragonfly takes off and climbs, in which the downstroke provides a lot of positive lift and drag, and the upstroke provides negative lift resistance. (ii) Counter stroking flight is the flight mode of the dragonfly when it is in stable and level flight, in which the positive and negative lift and drag of the fore and hind wings cancel each other out, so that the lift and drag curve is maintained at a low value, and the dragonfly can fly smoothly. (iii) No matter under any flight conditions, the average lift and drag of counter stroking flight is smaller than that in-phase stroking flight, and it can maintain enough lift to support body weight, indicating that counter stroking flight can keep the dragonflies stable.

Computational mechanics of soft matter and machines
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE THEORY AND SIMULATION METHOD OF THE ANISOTROPIC DAMAGE BEHAVIOR OF DOUBLE NETWORK HYDROGELS

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ABSTRACT

Double network (DN) hydrogels are a type of hydrogels composed of two interpenetrated polymer networks and water. It shows great potential to be applied in biomedicine and soft electronics areas etc., because of the superior flexibility and biocompatibility. In DN hydrogels, the first polymer network is crosslinked by shorter polymer chains and the second one is crosslinked by longer polymer chains. During the deformation of DN hydrogels, the polymer chains in the first polymer network are first straightened to fracture in succession, forming the microdefects, while the second polymer network with longer chains supports the bulk structure and reduces the stress concentration effectively. Thus, the toughening mechanism of DN hydrogels compared to single network hydrogels is to damage the first polymer network. Although current damage theories can capture the stress softening phenomenon of DN hydrogels, they encounter difficulties in describing and predicting the necking phenomenon of DN hydrogels, just because the multiscale mechanism of the damage behavior of DN hydrogels is still ambiguous. In this work, we conduct a multiscale investigation on the bottom-up damage mechanism, damage theory and simulation methods of DN hydrogels. We construct the random structural models of DN hydrogel in microscale using molecular dynamics methods at first. Then, the mesoscale topological network models are extracted from the microscale models with specific length and fracture criterion of every polymer chains. By developing a network mechanics method, we simulate the fracture of polymer chains and the damage of the mesoscale network models, and provide the damage behavior for developing macroscale anisotropic damage theories. The anisotropic damage theories are then numerically implemented by finite element methods. Our damage theories and simulation methods can reproduce the stress softening and necking phenomena effectively. This work provides insights on the multiscale damage mechanism of DN hydrogels and powerful simulation tool for mechanics design of DN hydrogels.

Multiscale modeling, analysis and numerical methods of material defect and inhomogeneities
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RIPPLOCATIONS IN GRAPHITE LAYERED COMPOSITES

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ABSTRACT

Layered structures involve the consolidation of single-layer materials through adhesive processing to solidify them into a layered form that meets specific structural requirements such as low weight, high strength-to-weight ratio, high stiffness-to-weight ratio, and fatigue resistance. The introduction of graphene nanosheets into a matrix to form layered composites can significantly improve the mechanical properties of the material. Therefore, graphite layered composites have great potential for various applications. However, at present, the theoretical calculation models for layered composites often overlook the commonly occurring interlayer deformation phenomenon and fail to effectively reflect the interlayer mechanical properties. We combine the mechanics and geometry to elucidate the deformation mechanisms of graphite layered composites.

In this study, molecular dynamics (MD) methods are used to describe the mechanical response and microevolution processes of graphite layered composite under tensile and compressive loading, revealing the microscopic evolution mechanisms that contribute to the differences in mechanical response under these two types of loading (1). At the same time, the effect of the number of graphene layers on the Young's modulus of the composite material is studied by observing the atomic structural changes under fracture conditions. During the compression simulation, kink and ripplocation deformation are observed, which are commonly generated in layered solids, but the deformation mechanisms are not clear. Due to the complex curved surfaces that occur during the compression simulation, the mean curvature and Gauss curvature based on the differential geometry methods are used to describe the non-uniform deformations (2). We calculate the external deformation of layered materials, and elucidate the reinforcement mechanism of graphene addition to the matrix and the deformation mechanism (3). The results show that ripplocation is a fully reversible elastic deformation, and it is found that ripplocation boundaries of the same sign integrate when compressed under certain conditions. Compared to existing studies, we are the first to use differential geometry methods to calculate the in-plane deformation of composites. This provides theoretical guidance for the design of high-strength, high-toughness graphite layered composites.

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Imaging-based methods in computational medicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ANALYZING TIME-LAPSE MICROSCOPY DATA TO QUANTIFY AND UNDERSTAND THE BEHAVIOR OF MECHANOBIOLOGICAL SYSTEMS

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ABSTRACT

From the beating heart to tissue assembly and repair, it is well accepted that mechanics plays an important role in the behavior of biological systems. Mechanical forces are not only fundamentally important to biological materials (e.g., the mechanics of growth), but are also fundamental drivers of cellular behavior change. However, it is often difficult to determine mechanical state both in vitro and in vivo, and it is often difficult to determine how mechanical perturbations (e.g., changes to boundary conditions) will change the mechanical state throughout the domain. Mathematical and computational modeling are important tools to bridge this gap, and image-based data is often the glue that connects mechanical theory to experimental data. In this talk, we will describe our preliminary and ongoing work in curating and disseminating microscopy data and software tools for data analysis and modeling. Specifically, we will focus on an ongoing project with collaborators in developing computational tools and mechanics based understanding of an in vitro three dimensional tissue model of wound healing. In brief, we envision a methodological framework with three essential components: (1) open access datasets of time-lapse movies of cells and tissue, (2) open source software to extract interpretable quantities of interest from these time-lapse movies, and (3) combined mechanistic and statistical models of biological behavior informed by these data. We are presently working on creating these datasets, software, and models in partnership with experimental collaborators, and releasing them to the community under permissive licenses. Looking forward, we anticipate that these large open access curated datasets combined with open source tools to extract information from them will enable significant advances in our understanding of, and ability to control, living systems. Through this talk, we hope to foster further discussion and collaborations at the interface of biomechanics, image analysis, and open science.

Imaging and computational methods for biomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE HEMODYNAMIC IMPACT OF INTRACRANIAL ARTERIAL STENOSIS AND THE CLINICAL IMPLICATIONS

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ABSTRACT

Intracranial arterial stenosis (ICAS) is a major cause of ischemic stroke around the world. It can cause an ischemic stroke by different mechanisms, e.g., the lesion (plaque) occluding the orifice of a branching artery to cause a single small infarction in the relevant territory, significant narrowing of the vessel lumen to cause hypoperfusion and possibly multiple infarcts in borderzone regions, and an unstable plaque to rupture and cause embolization of distal arteries and possibly multiple infarcts in the distal territory (cortical regions).

Presence of ICAS can impact focal and global hemodynamics. For instance, it is associated with elevated flow velocity and wall shear stress across the lesion and decreased pressure distal to the lesion, which can be affected by the morphology of adjacent arteries and the ICAS lesion. The hemodynamic impact of ICAS has important clinical implications, e.g., affecting the stroke mechanisms and risks in patients with ICAS. Those with significantly reduced pressure distally may have hypoperfusion, and those with significantly elevated wall shear stress may have increased plaque vulnerability and risk of plaque rupture and distal embolization. These both are associated with a higher risk of stroke relapse in patients with a first stroke due to ICAS, despite medical treatment recommended by clinical guidelines.

Therefore, studying the hemodynamic impact of ICAS has important value for stroke risk stratification in ICAS patients, based on which we can identify “high-risk” patients and design more effective treatment for stroke prevention.

16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Advances in discretization techniques, element technology, mesh adaptivity, and solution strategies for inelasticity, localization, and failure

July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ARBITRARY ORDER VIRTUAL ELEMENT METHODS FOR HIGH-ORDER PHASE-FIELD MODELING OF DYNAMIC FRACTURE

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ABSTRACT

Accurate modeling of fracture nucleation and propagation in brittle and ductile materials subjected to dynamic load is important in predicting material damage and failure under extreme conditions. The exact solution of the high-order phase-field fracture model has higher regularity. Thus numerical solutions of the model can embrace improved convergence and better accuracy. Virtual element methods are generalization of classical finite element methods and allow polytopal meshes. In this work, we develop a virtual element framework for the high-order phase-field model of dynamic fracture. We use H^1-conforming virtual elements and generalized-α method for the elastodynamic equation, and adopt H^2-conforming virtual elements for the high-order phase-field equation. We verify our virtual element framework using classical quasi-static benchmark problems and show numerical examples for dynamic fracture propagation.

Computational methods for wind energy
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFECTS OF OFFSHORE WIND ENERGY ON THE OCEAN CIRCULATION

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ABSTRACT

A one-way ocean-atmosphere coupling was developed to study the effects of offshore wind turbines on the surrounding oceanic regions. This was achieved by coupling the results of our in-house wind farm simulator UTD-Wind with FVCOM (unstructured Finite Volume Community Ocean Model). In the present study, Large Eddy Simulations were carried out to model the atmospheric boundary layer and wind turbines. The immersed boundary method was used to simulate the floating platform, tower, and nacelle, whereas the turbine blades were modeled using a rotating actuator disk model. The angular speed of the turbine was determined by the balance of aerodynamic and generator torque. The LES velocity fields were used as input by FVCOM to compute a space-time varying wind shear that served as forcing for the ocean model.

Numerical results show that wind turbines produce a low velocity wake region that impact the wind shear forcing acting on the sea surface current. Due to the wind shear gradient, upwelling is generated to counteract the lower velocity region underneath the turbine wakes. For conservation of mass, downwelling was produced in the adjacent regions of the turbine wakes, generating large vortices normal to the turbine rotor and across the depth of the domain. These results show the complex hydrodynamics occurring below offshore wind turbines. Potentially, these vortices could enhance the exchange of nutrients from the richer bottom of the ocean to the upper sea surface level. As a consequence, this could promote the growth of oceanic wildlife in the regions where the wind turbines are located.

This research contributes towards the wind energy field by utilizing numerical simulations to study the complex hydrodynamics occurring in the surroundings of offshore wind farms. It will be a large motivator to further study the presented research topic and explore how offshore wind turbines can positively impact the surrounding ecosystems. This topic can demonstrate the added benefits of developing offshore wind energy, not only because of its reduced carbon footprint, but additionally because of its positive environmental impact. In the long term, it could potentially contribute to making offshore wind a more dependable source of energy.

Modeling and simulation of dynamics, stability and control of aerospace structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A STUDY ON THE USAGE OF MAGNETO RHEOLOGICAL ELASTOMERS FOR NON-LINEAR AEROELASTIC OSCILLATIONS CONTROL

Henrique Edno Leoncini De Carvalho[*1], Reyolando Manoel Lopes Rebello da Fonseca Brasil[1], Matheus Silva Proença[2], Jeferson Camargo Fukushima[2], Daniel Henrique de Souza Obata[2], Fernanda Carolina de Almeida[2] and Amarildo Tabone Paschoalini[2]*

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ABSTRACT

Magneto Rheological Elastomers (MRE) are composite intelligent materials, which can substantially change their viscoelastic properties due to their high magneto-sensitivity in response to different regimes of external magnetic field. Under the influence of a magnetic field, both storage shear and loss factor of MREs increase, this field-induced phenomenon is often referred to as the magnetorheological effect. The practical application of MR materials demonstrates great potential for several areas, as indicates the increasing number of patents registered in the last decade. This research is included in a line aimed to develop MRE devices for structural vibrations' control, exploring the magnetorheological effect and its capacity to promote gains in viscoelastic properties, thus enabling changes of relevant magnitudes in structural systems, such as the natural frequency and damping ratio. This adaptive behavior can be studied by the analysis of qualitative numerical simulations, this study proposes to investigate the effectiveness of MRE devices on wind induced aeroelastic oscillations (galloping equation), the results are obtained by the Multiple Scale Method and numerical integrations, showing a trajectory suppression on the phase-plane of limit cycles to focal points, as well as a three-fold change in the critical speed and alterations on the shape of the Hopf’s bifurcation diagram.

Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GO-MELT: GPU-OPTIMIZED MULTILEVEL EXECUTION OF LPBF THERMAL SIMULATIONS

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ABSTRACT

Computationally modeling the melt pool in a part-scale LPBF model is expensive despite the fact that the laser only covers a small area within the entire domain. Hence, we developed GO-MELT, a multilevel approach inspired by VMS, to address this problem. To calculate the solution for a part-scale model, we couple three overlapping levels. In Level 1, we compute the coarse-scale temperature solution over the full domain. In Level 2, the meso-scale temperature solution that spans the melt pool region is solved. In Level 3, the fine-scale thermal solution in the immediate region around the laser is calculated. Subgrid scales are computed from both Levels 2 and 3. Overlapping meshes can track a moving laser for the full duration of the simulation without remeshing. As a result, GO-MELT can efficiently implement GPU acceleration using Google's JAX library with JIT compilation to significantly speed up the simulation. We conducted five case studies using GO-MELT to demonstrate proper convergence behavior, to show how fewer DOFs are required to reach the same accuracy as a uniform mesh, and to quantify execution time per timestep added per DOF in each level. Using GO-MELT, a simulated production run of a 10 mm cube required around 9.36 hours to complete 20.5 million time steps, averaging 1.64 ms per time step. For the same spatial resolution used in the melt pool region, GO-MELT is 678 times faster than a GPU-accelerated uniform mesh solver. We also demonstrate efficient simulation of a more complicated part geometry, including phase- and temperature-dependent properties that capture the effects of powder melting and fusion. Finally, we show that the fine-scale solution can be replaced by an alternative model, such as a data-driven surrogate model, giving the opportunity to further bridge simulation scales and improve both the speed and efficiency of part-scale LPBF simulations.

Scientific deep learning
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFICIENT SEMANTIC SLAM: LEVERAGING DEEP LEARNING FOR ENHANCED SLAM IN DRONE FORESTRY SURVEILLANCE UNDER CANOPY

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[1]*I2M*

ABSTRACT

This paper introduces an efficient approach for generating a real-time Simultaneous Localization and Mapping (SLAM) system using a stereoscopic camera mounted on a drone in an outdoor environment. Specifically, the study focuses on mono-species maritime pine forests, with an average spacing of four meters between tree rows. The primary objective is to generate a semantic map that accurately identifies the tree rows, enabling the automated estimation of an optimal trajectory that maximizes the distance between the rows to minimize the risk of collision. Standard Visual SLAM (VSLAM) algorithms, particularly those based on graph theory, are sensitive to lighting conditions because they identify, characterize, and re-associate landmarks across successive images. To operate effectively, VSLAM algorithms calculate a significant number of landmarks, enhancing robustness against occlusions and assignment errors.

In this presentation, we describe a rapid, efficient, and semantically-driven SLAM approach, leveraging object segmentation via deep learning. We have developed a robust and efficient image segmentation method that identifies nearby trees in each image. For these stationary objects, Kalman filter-based tracking techniques are employed to re-identify each tree throughout the video stream. A unique geometric feature, the centroid of each tree, is extracted and integrated into our graph-based SLAM algorithm. In this graph, each tree represents a single node, and the edges connecting different drone positions to a tree node represent depth estimations from the stereoscopic camera. Our method ensures a controlled graph size, maintaining compatibility with real-time operational scenarios.

To validate the effectiveness of the proposed method, it has been applied to real-world data collected from forest environments. This approach not only demonstrates the potential for more efficient and accurate environmental mapping but also represents a significant step forward in the application of AI and deep learning techniques in the field of robotic navigation and environmental monitoring.

Innovations in machine learning-enhanced uncertainty quantification for computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PROBABILISTIC CALIBRATION OF EXPENSIVE MODELS USING EFFICIENTLY TRAINED SURROGATES

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ABSTRACT

Calibration of computational models in the presence of uncertainty is often cast as a Bayesian inference problem and solved via sampling methods, e.g., Markov chain Monte Carlo. When the computational model is expensive, this task becomes intractable due to the large number of samples required to accurately estimate the posterior distribution of the calibration parameters. A popular solution to this problem is to use machine learning to develop a faster-to-evaluate, lower-fidelity substitute for the original model to serve as a surrogate while solving the inference problem. Although considered an offline cost, generating training data to construct this surrogate model can still be an expensive task in practice.

An active learning algorithm is presented that focuses training on improving surrogate accuracy specifically in and around the bulk of the posterior distribution, as this is where the model is exercised during calibration. Candidate samples are drawn from families of distributions related to an approximation of the posterior. The sample maximizing predictive variance is then selected for evaluation by the original computational model, yielding a label for the training point. Iterating this approach increases efficiency relative to space filling designs (e.g., Latin hypercube sampling) by avoiding low probability points. Practical considerations are discussed, including the benefits of using a sequential Monte Carlo sampling approach, convergence heuristics, and the importance of both exploration and exploitation given that the true posterior is unknown a priori.

Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN SURROGATE MODELLING OF RESIDUAL STRESSES IN LASER POWDER-BED FUSION

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ABSTRACT

In order to enable the industrialization of additive manufacturing, it is necessary to develop process simulation models that can rapidly predict part quality. Although multi-physics simulations have shown success at predicting residual stress, distortion, microstructure and mechanical properties of additively manufactured parts, they are generally too computationally expensive to be directly used in applications, such as optimization, controls, or digital twinning. In this talk we present a critical evaluation of how data-driven surrogate models can be used to model the residual stress of parts fabricated by Laser Powder-Bed Fusion. Three different models using varying levels of sophistication are compared: a multilayer perceptron (MLP), a convolutional neural network (CNN) based on the U-Net architecture, and an interpolation-based method based on mapping geometries onto a reference. All three methods were found to be sufficient for part design, providing mechanical predictions for a CPU time below 0.2 s, representing a runtime speed-up of at least 3900 × . Neural network-based models are significantly more expensive to train compared to using interpolation. However, the generality of models based on the U-Net architecture is attractive for applications in optimization.

OPTIMAL PATH PLANNING FOR LPBF AS AN EQUALITY GENERALIZED TRAVELING SALESPERSON PROBLEM

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ABSTRACT

Planning a laser path in Laser Powder Bed Fusion (LPBF) printers may benefit from being optimized to improve certain conditions for a print, such as minimizing a measure for the induced temperature gradients with the hope it is correlated with residual stresses, or increasing the overall time each part of a print remains hot to partially temper it. The simplest version of this problem discretizes the laser path as a sequence of tiles and aims to determine the order in which the tiles are to be heated by the laser.

In this talk we show that the problem of determining an optimal tile ordering can be reduced to an Equality Generalized Traveling Salesperson Problem (E-GTSP), a reduction that opens the problem to be solved through commonly used heuristics. We then demonstrate the performance of this identification towards solving some simple LPBF path planning problems.

A STABLE HYPERELASTIC MODEL FOR FOAMED RUBBER OVER A LARGE RANGE OF POROSITY

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ABSTRACT

A hyperelastic model for foamed rubber is presented. The model is a modification of the CHIPFoam (Compressible, Hyperelastic, Isotropic, Porosity-based Foam model) model. The strain energy is in terms of the first isochoric invariant, $\bar{I}_1$, of the Cauchy-Green tensors and the relative volume, J. The model includes a function that couples deviatoric and volumetric deformation. The onset of this coupling function may be delayed based on the porosity of the foam or on the morphology of the porosity. The relative volume is multiplicatively decomposed into a part derived from isochoric deformation of the rubber and a part resulting from compressibility of the rubber.

In addition to this delayed action of the pore compression function, the volumetric buckling function in CHIPFoam was modified. This modification leads to a more stable and more easily converged response.

The model may be applied for foams with initial porosities that range from less than one percent to porosities of greater than 99 percent. The model includes a simple elastic damage model for an elementary form of cyclic softening. It does not include any other dissipative deformation mechanisms. It is therefore only appropriate for materials with very little hysteresis or for monotonic loading only.

The model basis and examples of model fits to a variety of foams will be presented. Additionally, some thoughts on the inclusion of viscous deformation effects will be discussed.

Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MESH ADAPTATION FOR FREE SURFACE FLOW SIMULATIONS USING THE PARTICLE FINITE ELEMENT METHOD

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ABSTRACT

The Particle Finite Element Method (PFEM) [1] is a strong approach for simulating free surface flows, fluid-structure interactions (FSI), and other applications featuring highly deformable domain geometries. A hybrid method that seamlessly integrates Eulerian-based solvers and particle methods, PFEM takes advantage of both approaches. In essence, PFEM represents the fluid using a set of particles, which are triangulated at each time step to construct a mesh. The conservation equations are then solved on this mesh through the finite element method, yielding the material velocity for each particle. Subsequently, using this velocity information, the particle positions are updated, resulting in a dynamically deformed domain that is triangulated again in the following time step.

Central to the PFEM's effectiveness is the need to detect domain boundaries, a key aspect that also presents one of its primary challenges. Given that the particles are triangulated again in each time step, the shape of the fluid domain requires continuous redefinition. This necessitates the use of an indicator function to discern the fluid's shape, akin to the challenge of detecting the shape of a point cloud. By combining the alpha-shape algorithm, initially proposed by Edelsbrunner [2], with a mesh adaptation step based on Delaunay refinement algorithms [3], we enhance the overall method. This approach demonstrates consistency, particularly in terms of addressing the significant challenge of volume conservation inherent in Lagrangian methods.

Our study will present comprehensive results in both 2D and 3D for free surface flows, showcasing advancements and demonstrating the efficacy of our method. Additionally, we will explore aspects of coupling with other discretisation methods, such as discrete element methods and solid mechanics finite elements, particularly in the simulation of FSI problems.

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Recent advances in computational fracture mechanics and failure analysis
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ANALYSIS OF THERMOMECHANICAL DELAMINATION MECHANISMS IN SEGMENTED HIGH-TEMPERATURE PROTECTIVE COATINGS AND DESIGN MAPS FOR THE DURABLE COATINGS

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ABSTRACT

Protective coatings play a crucial role in preserving high-temperature engineering components from environmental degradation. The durability of these coatings is crucial for maintaining the structural integrity of the components. Introducing a segmented microstructure was recognized as an effective strategy for enhancing the strain tolerance of coatings by mitigating the in-plane stiffness of the coatings, thereby alleviating interface stresses and delamination driving forces. While previous studies on delamination mechanisms in high-temperature protective coatings have predominantly focused on either pure mechanical loading or pure thermal loading conditions (i.e., residual stress) due to their ease of implementation, the combined influence of both loads remains relatively unexplored. This work systematically studies delamination problems in segmented multilayered high-temperature coatings subjected to thermomechanical loadings using computational fracture mechanics. A representative unit cell model is introduced, which is used to analyze coatings over a broad range of material properties, geometries, and loads. The findings suggest that, for a given coatings system, the mechanical load carried by the top-coat layer is the only force driving delamination along the top-coat/bond-coat interface. A mathematical model is established using combined multiple regression analyses and the design of experimental method to evaluate the delamination driving forces and rank the importance of various influential factors. Design maps are constructed to facilitate the development of durable coatings.

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Battery modeling and computation: From material to device
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

REACTIVE DIFFUSION OF LITHIUM IN SILICON – NEW INSIGHT FROM ATOMISTIC SIMULATIONS

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ABSTRACT

Atomistic simulations are performed to investigate the insertion of lithium (Li) in crystalline silicon (c-Si) by using a modified embedded atom method potential. The mechanism for the formation of the amorphous a-LixSi was analyzed by conducting novel structural analysis. Diffusion pathways of Li in c-Si and the energy barrier are also analyzed and calculated. The results show that Li atoms diffuse preferably along the 112 directions on the {111} planes, and the energy barrier is too high for thermally activated diffusion around room temperature. The formation mechanism for the amorphous/crystalline interface (ACI) is also analyzed. The diffusivity of Li in Si is calculated based on the simulation results. Our results show that the diffusivity of Li in the a-LixSi is about 50~100 times faster than in the c-Si. Our results also show that the composition of Li in the a-LixSi is non-uniform during lithiation, and the distribution of Li is analyzed. The simulation results are compared with the available experimental results.

The phase field method for fracture: Theory, numerics, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STABILIZED FORMULATION FOR PHASE-FIELD FRACTURE IN NEARLY INCOMPRESSIBLE HYPERELASTICITY

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ABSTRACT

This work presents a stabilized formulation for phase-field fracture of hyperelastic materials near the limit of incompressibility. At this limit, traditional mixed displacement and pressure formulations must satisfy the inf-sup condition for solution stability. The mixed formulation coupled with the damage field can lead to an inhibition of crack opening as volumetric changes are severely penalized effectively creating a pressure-bubble. To overcome this bottleneck, we utilize a mixed formulation with a perturbed Lagrangian formulation which enforces the incompressibility constraint in the undamaged material and reduces the pressure effect in the damaged material. A mesh-dependent stabilization technique based on the residuals of the Euler–Lagrange equations multiplied with a differential operator acting on the weight space is used, allowing for linear interpolation of all field variables of the elastic subproblem. This formulation was validated with three examples at finite deformations: a plane-stress pure-shear test, a two-dimensional geometry in plane-stress, and a three-dimensional notched sample. In the last example, we incorporate a hybrid formulation with an additive strain energy decomposition to account for different behaviors in tension and compression. The results show close agreement with analytical solutions for crack tip opening displacements and performs well at the limit of incompressibility.

Multiscale modeling, analysis and numerical methods of material defect and inhomogeneities
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL SIMULATION OF MATERIAL STRENGTH OF CMCS BASED ON CT DATA RECONSTRUCTION

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ABSTRACT

Ceramic-Matrix-Composites are an important material candidate for thermal structures in aero engines. To investigate the strength failure of CMC materials occurring at ordinary temperature service, this paper establishes a detailed geometric model of the material by obtaining the material structure and defect distribution characteristics through CT technology and establishes a strength prediction model of ceramic matrix composites at ordinary temperature by writing different material subroutines for the failure modes of different kinds of materials.

First, we carried out the geometric analysis model and FEM model construction for 2D-C/SiC composites containing defects. Using μX-CT technique, we conducted CT scans on four specimens of 2D-C/SiC composites at different locations and sizes, respectively. Based on the CT slice data obtained from the scans, the volume fraction and location distribution of defects were obtained by reconstructing and analyzing the material defects. Meanwhile, by analyzing the CT slice data, we obtained the geometric parameters of fiber bundles in 2D-C/SiC composites, characterized the geometry of fiber bundles more accurately, and placed the hole-type defects completed by the analysis into them, and finally obtained the single-layer finite element analysis model of 2D-C/SiC composites and the structural FEM of 2D-C/SiC composites.

Next, numerical simulations of the strength of 2D-C/SiC composites were performed. Based on FEM, the fiber bundles consisting of fibers and matrix are equated to a homogeneous material by the known use of the equivalent homogenization method. By writing the VUMAT subroutine, we defined the fiber bundle failure criterion and the matrix failure criterion respectively, and simulated the static tensile process of the material. In the simulation, we found that during the static stretching of the material, the damage of the material occurs first below the location of the coating cracks, and the cracks gradually expand downward with the increasing tensile load. After the failure of the first layer, the crack expansion path changed clearly from directly below the coating crack defect to the maximum bending position of the woven structure, which is more in line with the crack expansion law of CMC material in the static tensioning process. Through the numerical simulation analysis of the static tensile strength of the material at room temperature, the tensile strength of the material at room temperature was determined, and the reliability of the finite element model was also verified by combining the test results. This supports the effective data for ceramic matrix composites in material design and engineering applications.

Uncertainty quantification and reliability analysis in engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RELIABILITY ANALYSIS OF CABLE-STAYED BRIDGE SYSTEM BASED ON DIRECT PROBABILITY INTEGRAL METHOD

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ABSTRACT

The system reliability analysis of cable-stayed bridges is an important part of structural safety analysis, and this paper proposes a method to analyze the overall dynamic reliability of prestressed concrete cable-stayed bridges based on the direct probability integral method. Firstly, the limit state equations of the main girder bending strength failure, wind-induced vibration failure and the main tower strength damage failure in the downward direction and the transverse direction buckling failure as well as the strength damage failure of the tie ropes of the cable-stayed bridge are established. Then the reliability analysis of the whole bridge cables is carried out, and the most dangerous three pairs of cables are selected to form a series-parallel system with the failure modes of the main girders and towers of the cable-stayed bridge, and the joint probability density integral equations of the extreme value mapping of multiple performance functions are established. Finally, the equations are solved using the direct probability integration method containing Heaviside function (DPIM-H) to obtain the overall dynamic reliability index of the cable-stayed bridge, and the Monte Carlo method is used to verify the reasonableness of the results. Taking the prestressed concrete cable-stayed bridge as an example, the system degree is analyzed by DPIM-H as well as the reasonableness of the results is verified by Monte Carlo.

Multiphase flow and non-Newtonian fluid - Modelling and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PORE-SCALE STUDY OF MULTIPHASE FLOW PATTERNS IN LAYERED POROUS MEDIA WITH FRACTURES

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ABSTRACT

The presence of fractures increases the difficulty of multiphase flow mechanism analysis, and it remains unclear how fractures affect multiphase flow displacement in the layered rock matrix. Herein, a pore-scale imbibition model considering the layered matrix-fracture system is established using the phase-field method, where oil is displaced by a range of fluids with various properties. Two typical flow modes are carefully analyzed, depending on the locations of the fracture and the interfaces between different layers of the matrix: fracture is parallel to the interface (mode I) and it penetrates through the interface (mode II), which are dominated by the co-current imbibition and counter-current imbibition mechanisms, respectively. Interestingly, the surface tension is found to be negatively correlated with the ultimate oil recovery rate for mode I and plays an opposite effect on that of mode II. For flow mode I, the conditions of lower injection rate, higher viscosity ratio, higher grain diameter ratio, and injection of the invading fluid from the larger pore throat size (positive direction flow) can improve oil recovery. For flow mode II, the fracture bifurcation angle has little effect on the positive direction flow, while it can significantly regulate the phase distribution in the negative direction flow. Based on the scaling analysis of relating pore-filling events to displacement modes and the equilibrium relationship between capillary and viscous forces, two theoretical models are derived to predict the imbibition patterns, and the variation of the flow regime under various parameters in the typical layered matrix-fracture models is systematically concluded.

Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMAGE-BASED MESOSCOPIC SIMULATIONS OF ALLOYS

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ABSTRACT

Polycrystalline materials consist of aggregates of grains with varying lattice orientations and sizes separated by grain boundaries. The random morphological and crystallographic microstructure characteristics are responsible for the anisotropic behavior of polycrystalline microstructures and determine their macroscopic properties and performance. The mechanical properties of alloys, including stress and strain response and elastoplastic anisotropy, are significantly affected by morphological and crystallographic (grain orientation, etc.) features.

The present studies of the microstructure effect on mechanical properties and performance have certain limitations. Research methodologies are mainly limited to representative volume elements (RVEs)-based experimental observations. In practice, the microstructure characterizations exhibit a large degree of randomness during deformation processing, and microstructure randomness reveals polycrystalline materials' probabilistic properties and performance. Consequently, the vast size and number of the microstructure RVE necessary to build the process–structure–properties–performance (PSPP) linkages are computationally prohibitive and challenging to investigate. Meanwhile, the simplified polycrystalline microstructures, such as single crystals, bicrystals, Voronoi, and ellipsoid polycrystals, fail to capture all the statistical microstructure characterizations of the heterogeneous grains. Aa a result, the datasets between microstructural characteristics and mechanical properties and performance are unlikely to be built without sufficient data.

In this work, we propose a patch-based texture synthesis reconstruction algorithm to accurately capture the statistical microstructure characterizations of the heterogeneous grains. Then, the established computational plasticity FEM model combined with explicit characterization algorithms was used to perform quantitative analysis on Inconel 718 superalloy to fully understand the macroscopic properties and performance responses (ultimate tensile strength, Von Mises stress, ductile failure initialization and propagation) in terms of morphological, crystallographic, and boundary characteristics. Finally, the patch-based texture synthesis coupled with explicit characterization algorithms was developed to determine the ductile failure sets using the microstructural parameters, such as grain orientation and boundary characters.

Modeling friction and wear
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LOAD-AREA RELATION OF RANDOM ROUGH SURFACES FOR LARGE CONTACT FRACTION

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ABSTRACT

Establishing the accurate load-area relation is pivotal for comprehending complex phenomena such as friction, wear, and thermal and electrical conduction, particularly for large contact fraction. Unfortunately, prevailing contact models often fall short in capturing behaviors across the entire contact regime due to the oversight of intricate asperity interactions, especially in high load level. In this investigation, we address the challenge by incorporating asperity interactions in both elastic and elastic-plastic contact. The actual random distribution of contacting spots with various sizes is simplified as a hexagonal distribution of identical spots sharing the same quantity and total area. Leveraging the perfect symmetry, a representative asperity is then simulated by finite element method and asperity interaction is incorporated through the periodic boundary condition. The load-area relation is calculated up to almost complete contact. It is interesting to find that surface morphology and material properties predominantly affect the initial linear relation at small contact fraction, and the interactions among asperities are closely related to contact fraction and lead to a larger load than that neglecting asperity interactions. By comparing with the theoretical prediction of an incremental equivalent contact model at initial contact, the load-area relation is extended for general rough surfaces. Direct simulations on typical rough surfaces verify the accuracy of the advanced load-area relation within a large range of contact fraction. This developed model provides an efficient method to predict the overall contact response of rough surfaces, significantly reducing the computational burden. The advancement serves as a robust foundation for in-depth analyses in tribology, laying the groundwork for a nuanced understanding of friction, wear, and sealing behaviors.

Boundary element methods: New theories and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BI-MATERIAL TOPOLOGY OPTIMIZATION FOR VIBRO-ACOUSTIC PROBLEMS BASED ON NON-NEGATIVE INTENSITY

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ABSTRACT

In this work, the non-negative intensity (NNI) method is applied to a large-scale vibro-acoustic interaction system using the fast multipole boundary element method (FMBEM), and a bi-material topology optimization method is constructed to minimize the integration of non-negative intensity on predefined surfaces. The NNI provides a field on the surface of the radiating structure, consisting of positive-only contributions to the radiated sound power, which avoids the near-field cancellation effects that otherwise occur with the sound intensity field [1]. To intuitively characterize the contribution degree of structural surface to far-field radiation and provide a theoretical basis for acoustic radiation analysis and design of large-scale vibro-acoustic interaction systems, the FMBEM is adapted to the NNI by calculating the eigenvalue solution of the symmetric acoustic impedance matrix using a two-stage solution method. The fast multipole algorithm is adapted to accelerate the calculation of matrix vector products of adjoint problems. The topology optimization of a large-scale submerged cylindrical shell model is realized using FMBEM [2]. The vibro-acoustic interaction system is first solved using a FEM–FMBEM model, and the resulting surface fields are then used in the FMBEM calculation of the NNI. The integration of the NNI on the predefined surface is selected as the objective function to design the radiation mode of the structural surface. A structural material interpolation model is established using the solid isotropic material with the penalization method, and the topological sensitivity formulation is derived based on the adjoint variable method. Numerical results confirm the effectiveness of the proposed optimization method in minimizing the integration of the non-negative intensity.

Keywords: FEM-FMBEM coupling analysis; topology optimization; non-negative intensity

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MULTI-PHYSICS FRACTURE ANALYSIS OF COMPOSITE LAMINATES BASED ON EXTENDED LAYERWISE METHOD

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ABSTRACT

An extended layerwise method (XLWM) is presented for the composite laminates with multiple delaminations and transverse cracks. The discontinuity of displacements and temperature induced by multiple delaminations is simulated by strong discontinuous function while the discontinuity of strain between dissimilar layers is modeled by a weak discontinuous function. Transverse cracks are modeled using classical Extended Finite Element Method (XFEM). And then, based on the XLWM, some mixed variational principle is employed or presented to derive the Euler equations and the discrete forms for the multi-physics fracture analysis of composite laminates. A fully coupled time integration method is developed based on the Newmark integration algorithm and Crank-Nicolson scheme, the multi-physics fields are solved simultaneously. The thermo-mechanical, thermo-chemo, thermo-chemo-mechanical, piezoelectric-mechanical, thermo-piezoelectric-mechanical and thermo-mechanical-curing-seepage coupling analysis are carried out numerically for the damaged composite laminates. Many numerical examples are studied to demonstrate the capabilities of static response, stress intensity factor and energy release rate for the composite plates, stiffened plates and sandwich plates.

Multi-scale, multi-rate damage and fracture: Models, experiments, and simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CREEP LIFE MODELLING OF NICKEL-BASED SINGLE CRYSTAL SUPERALLOY DD6 WITH MCRALY COATING

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ABSTRACT

Single-crystal superalloy is a crucial structural material widely employed in aerospace, energy, and petrochemical industries. High-temperature creep resistance is a critical indicator for evaluating alloys. In this study, a method for predicting the creep behavior of MCrAlY-coated DD6 single crystal alloy was proposed, and the influences of oxide layer thickness and inner wall temperature on the creep strain rate were investigated. The model was validated experimentally. The results indicate that the MCrAlY coating has a minimal impact on the high-temperature creep lifetime of [001]-oriented DD6 single-crystal superalloy. Pre-exposure treatment thickens the initial oxide layer of the coating, effectively extending the creep lifetime of the coated alloy, particularly at higher temperatures and stress levels. This underscores the effectiveness of pre-exposure treatment in increasing the creep lifetime of the MCrAlY-coated DD6 single-crystal superalloy system. The influence of inner wall temperature on creep lifetime follows a parabolic pattern. Excessively low inner wall temperatures reduce creep lifetime due to significant thermal mismatch stresses, while excessively high inner wall temperatures decrease creep lifetime because of changes in material properties at those temperatures.

Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TYPE Ⅰ TO TYPE Ⅱ TRANSITION IN SWEPT-FORWARD FIN SHOCK INTERACTIONS

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ABSTRACT

The transition from Type I to Type II in the swept-forward fin shock interaction is important, as it represents a shift from low to high heat flux interaction types. However, the mechanism for this transition remains unclear. In this study, theoretical and numerical analyses is employed to explore the transition mechanism. A theoretical model is developed to obtain the analytical solution for the transition condition, considering only the interaction of the incident shock and the bow shock of the fin on the symmetry plane. The theoretical solution is compared with numerical results at a freestream Mach number of 6.36. The results suggest that the transition occurs advanced, with three distinct transition mechanisms observed. At small wedge angles, the downstream flow pattern has an influence on the transition. In the downstream flow, the transmitted shock reflects on the wall as a Mach reflection. If the height of the Mach stem approaches the detachment distance of the fin shock, the transition occurs. At larger wedge angles, the transition occurs when the Mach number behind any one of the two transmitted shocks is less than 1. The other transition is observed at a wedge angle of 30°, which occurs accompanied by the disappearance of the supersonic jet.

Applications of shape optimization in complex engineering problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SHAPE OPTIMIZATION FOR LITHIUM-ION BATTERY WITH POROUS ELECTRODES

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ABSTRACT

In this presentation, we introduce a gradient-based shape optimization framework to design porous electrodes for maximum energy storage. Lithium-ion batteries are becoming increasingly important energy storage devices. Highly tortuous electrode materials can provide significant surface area per volume, which is required for large energy density. However, such a tortuosity can also deteriorate electrochemical transport, leading to poor material utilization in planar electrodes. Consequently, architecting electrodes that account for both transport and chemical activity is a promising alternative.

We consider a model with two materials: porous electrode and pure electrolyte. Density-based topology optimization has previously been used to design batteries for both half-cell and full-cell models to maximize energy storage. Despite the capability of producing complex interdigitated structures, an appropriate penalization scheme for intermediate materials is required for the optimizer to provide near binary designs. Setting up such a penalization is often time-consuming due to the large number of design-dependent variables that affect the forward model differently. Alternatively, the shape optimization approach used in this work produces binary designs naturally by morphing conformal meshes, circumventing inaccuracies associated with fuzzy interfaces. Shape sensitivities are computed via the adjoint method and leveraging automatic differentiation. The optimization problem is solved using a nonlinear programming technique.

In this presentation, we perform shape optimization on a half-cell model to maximize its energy storage when a fixed charging current is applied. We study multiple arrangements of physical parameters and compare their performance against a monolithic electrode. Both 2D and 3D results are presented.

Recent advances in computational fracture mechanics and failure analysis
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STUDY OF TIMOSHENKO BEAM-BASES CRANKSHAFT MODEL WITH NON-LINEAR BREATHING CRACKS

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ABSTRACT

With the development of the marine industry, marine diesel engines have the characteristics of complex structure and worse operating environment and frequently changing operating conditions, which put forward higher requirements on the index of shaft vibration. In the actual operation of a diesel engine, the crankshaft will generate three forms of vibration: bending, axial and torsion. These three forms of vibration are coupled with each other. Therefore, it is studied of the three-dimensional coupled vibration problems of the crankshaft system in this paper.

Firstly, the single crank is simplified as a five-segment straight beam structure. Based on the continuum vibration theory, the three-dimensional space field transfer matrix of the straight beam is derived. It is established for the point transfer matrices of coordinate transformation by using the conditions of displacement continuity and force equilibrium. The three-dimensional coupled vibration dynamic equation of the crankshaft system is constructed by using the multiplication of the transfer matrices. By taking modalities as generalized coordinates, there are simple representation for kinetic energy and potential energy of the vibration system. Lagrange equation is used to establish the differential equation of forced vibration of Simple crank system. The response of three-dimensional coupled forced vibration can be solved. A Timoshenko beam-based modelling method is proposed in this study, which considered the cross-section shape effect of the beam and non-linear breathing cracks are inserted as a spring potential energy term of the Lagrange equation.

Secondly, the finite element model of the crankshaft system was built by ANSYS WORKBENCH. The free vibration and forced vibration of the crankshaft system are calculated. The coupling vibration characteristics of the crankshaft system with non-linear breathing cracks under the burst force are analyzed. The results verified the correctness of the theoretical method in this paper.

Machine learning and data driven based engineering computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN MODELLING AND OPTIMIZATION METHOD FOR EFFICIENT MODELING OF COMPLEX STIFFENED CURVED SHELLS

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ABSTRACT

A data-driven modelling and optimization method is proposed to automatically model and optimize stiffeners on the complex stiffened curved shells. Firstly, a novel mesh-mapping method is developed for the data-driven modelling of complex stiffened curved shells based on radial basis function surrogate model. Secondly, an active learning-driven control point optimization method is proposed, which can improve the efficiency of modeling. Furthermore, a data-driven optimization approach, based on the deep neural network method, is employed to minimize the weight of the complex stiffened curved shells. Finally, two engineering examples are presented to verify the effectiveness of the proposed method, which reduces the modeling time by 84.9% and 66.3%, respectively, compared to using all control points in mesh-mapping. In conclusion, the proposed method has substantial potential in efficient modeling and improving engineering’s optimization efficiency.

Fracture, damage and failure mechanics of cementitious materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INVESTIGATION OF MESOSCALE FRACKING IN HETEROGENEOUS QUASI-BRITTLE MATERIALS USING A HYDROMECHANICAL COHESIVE PHASE-FIELD MODEL

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ABSTRACT

This study develops a mesoscale hydraulic fracturing modelling method combining a hydromechanical cohesive phase-field model with random field (RF) models and random aggregate models for simulating complicated 2D/3D mesoscale hydraulic damage and fracture in quasi-brittle materials. In this method, a Weibull RF generation algorithm is used to implicitly represent the material's fracture properties such as tensile strength and fracture energy, and its meso-structures such as aggregate, mortar, and interfaces are explicitly built using a random aggregate generating and packing algorithm and an aggregate scaling algorithm. The hydromechanical cohesive phase-field model is used to automatically model fluid-driven crack initiation and propagation in mesoscale models without remeshing. Monte Carlo simulations and parameter studies are then carried out to investigated the effects of mesoscale properties on fracking. A concrete cube under hydraulic pressures was analysed as an example. It is found that the predicted crack paths and fluid pressure curves both are stochastically affected by random fracture properties. A higher variance of tensile strength leads to a lower mean and larger standard deviation of peak pressures. Due to weaker fracture properties of aggregate-mortar interfaces than mortar, 3D hydrocrack tends to propagate along interfaces, leading to tortuous and non-planar crack paths after fracking.

CONFINEMENT EFFECTS ON THE THERMODYNAMICS AND FLUID FLOW IN POROUS MEDIA

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ABSTRACT

Unconventional shale recovery requires fundamental understandings of confinement effects on fluids flow behavior. Natural shales have complex pore network and chemical compositions, which prevent systematic study to understand the confinement effects. In this talk, we will present results from molecular simulations and provide insights into pressure-driven hydrocarbon fluid flow confined under amorphous silica pores. Coarse grained molecular simulations are performed to elucidate how confinements including the confinement size, shape, surface wettability, influence the thermodynamics and fluid transport in pores of single nanometer size. The force parameters of the adopted coarse grained molecular model are calibrated from the thermodynamic equation of state. Our numerical results demonstrated the importance of fluid-pore interaction, pore size, and pore morphology effects in mediating the pressure-volume-temperature (PVT) properties of hydrocarbons. Also, we found that the saturation pressure predicted from the van der Waals-type adsorption isothermal loop could be elevated or suppressed relative to the bulk phase. Based on the flow simulation results, a detailed analysis regarding the impact of each of these factors will be presented.

Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATION OF SOLID SHELL MATERIAL POINT METHOD IN EXTREME DEFORMATION OF THIN STRUCTURES

Jiasheng Li[*1] and Xiong Zhang*[1]

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ABSTRACT

Shell structures play a significant role in large-span situations. For safety and security, large deformation and destruction of shell structures has attracted great attention. With the large span of shell structures and inhomogeneous in material distribution, experiments of equal proportion are ordinarily expensive, while the corresponding results of the same experiment conditions may vary from each other. Therefore, the development of efficient and powerful algorithms to simulate complicated responses of shell structures remains an active field of research.

The standard material point method (MPM) has been applied to simulate shell structures. Several locking phenomena induced by the linear shape function will result in an overestimation of stress state and an underestimation of deformation when adopting a coarse background grid in the standard MPM. And thus, the discretization size of background grid should be small enough for shell simulations with the standard MPM, usually smaller than 1/5 of the shell thickness, which would lead to prohibitive computational cost.

A novel solid-shell material point method (SSMPM) is proposed in this work by introducing shell particles and locking treatments. The SSMPM adopts the shell particles to define the geometry of shell structures. A shell particle consists of a hexahedral particle domain, eight corners and Gauss quadrature points. Its deformation is obtained by solving the momentum equations on the background grid. For each shell particle, the assumed natural strain (ANS) method is adopted to eliminate shear locking and trapezoidal locking, and the enhanced assumed strain (EAS) method is employed to eliminate thickness locking. With the accurate description of bending modes, a single layer of shell particles and a coarse background grid are sufficient for shell structure simulations, which dramatically increase the computational efficiency. A local multi-mesh contact method is presented for contact situations. The advantages of MPM particles to simulate fragmentation and shell particles to simulate bending deformation are combined for extreme deformation of thin structures.

DEVELOPING AND ANALYZING A NOVEL UNCONDITIONALLY STABLE EXPLICIT FINITE ELEMENT METHOD FOR THE ELECTROMAGNETIC ROTATION CLOAK MODEL

Yunqing Huang[1], Jichun Li[2] and Bin He[3]*

[1]Xiangtan University
[2]University of Nevada Las Vegas
[3]Lanzhou Jiaotong University

ABSTRACT

One potential application of metamaterials is for designing invisibility cloaks. In this talk, I'll talk about a rotation cloak model. Here we carry out the mathematical analysis of this model for the first time. Through a careful analysis, we reformulate a new system of governing partial differential equations by reducing one unknown variable from the originally developed modeling equations in our previpous work [1]. Then a novel unconditionally stable explicit finite element scheme is proposed and its stability and optimal error estimate are proved. Numerical simulations are presented to demonstrate that the new scheme for the reduced modeling equations can effectively reproduce the rotation cloaking phenomenon. The talk is based on [2].

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Uncertainty quantification and reliability analysis in engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RESEARCH ON THE DYNAMIC RESPONSE OF OIL STORAGE TANK PLATFORM STRUCTURE UNDER THE EARTHQUAKE ACTION IN ICE REGIONS

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ABSTRACT

In recent years, with the rapid development of China's economy, the importance of marine resources has become increasingly prominent. Oil storage tank platform structures play a fundamental role in the development of offshore oil and gas resources. These structures often face complex and harsh environments in ice-prone regions, including the threat of seismic excitation and seasonal sea ice. To ensure the safe operation of offshore platform structures, it is necessary to conduct research on the dynamic response of oil storage tank platforms in ice zones under seismic excitation. In addressing this issue, this study developed a non-freezing model ice that is representative of the Bohai Sea ice environment. Subsequently, underwater vibration table tests were conducted on the oil storage tank platform structure using the model ice in a model ice pool. A numerical model was also established to simulate the dynamic response of the oil storage tank platform structure under seismic excitation. The seismic response analysis of the oil storage tank platform structure in ice zones was conducted by combining the numerical model and experimental data.

Multiphysics biomechanics of bio- and bio-inspired soft materials: Theory, simulation and experiments
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SELECTIN AND INTEGRIN COOPERATIVELY REGULATE ROLLING ADHESION OF LEUKOCYTE UNDER SHEAR FLOW

Long Li[1] and Jizeng Wang*[1]

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ABSTRACT

Cell interacting with its extracellular matrix involves complex structures formation consisting of a multitude of proteins and often takes place in a hydrodynamic environment, e.g., leukocyte locomotion inside blood vessel in the process of inflammation. Despite the omnipresence of rolling adhesion of cell mediated by multiple type of proteins under hydrodynamic impact, the mechanisms underlying how the mechanics of multiple proteins cooperatively may govern the dynamics of cell rolling is not yet fully resolved. Here we present a mechanical model on rolling adhesion of cell mediated two distinct adhesive proteins in shear flow, corresponding to selectin- and integrin- jointly regulating leukocyte adhesion. Considering two pairs' binding/unbinding events as Markov processes and describing kinetics of leukocyte by the approach of continuum mechanics approach give rise to the mechanical description of rolling adhesion process. Through examining the dynamics of leukocyte rolling as a function of relative fraction of selectin and integrin pairs, we show that, during recruitment, the elongation of intermittent weak selectin bonds consuming the kinetic energy of rolling leukocyte decelerates the rolling speed and enables the integrin pairs to form strong bonds, therefore achieving the arrestment of leukocyte (firm adhesion). The coexistence of selectins and integrins may also be required for effective phase transition from firm adhesion to rolling adhesion, due to dynamic competition in pairs' formation and elongation.

Lattice Boltzmann modelling and study of complex flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL STUDY ON THE INNER WETTING MECHANISM FOR HYDROGEN-OIL SYSTEM IN THE POROUS MEDIA OF THE CATALYST PARTICLE WITH DIFFERENT SHAPE BASED ON THE PF-LBM

MengHui Li[12], Yumei Yong[2], Hanyang Mo[23], Wenqiang Chen[24], Jialin Dai[24] and Chao Yang[2]*

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[3]*China University of Mining and Technology-Beijing*
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ABSTRACT

The inner wetting characteristics in the catalyst particles have a significant impact on the activity and selectivity of catalysts[1]. Due to the complexity of the internal geometry structure of particles and the limitations of experimental conditions, the wetting condition inside particles remains unknown and assumed. Therefore, the paper numerically explored the wetting state and mechanism for hydrogen-oil flow in a catalyst particle by phase field lattice Boltzmann method (pf-LBM) developed by our team[2]. First, we randomly constructed irregular pore structures and reproduced the cross-sectional morphology of the catalyst particles. Combining the uniform distribution and Gaussian distribution, using the Voronoi edge topology to take the midpoint, doing spline interpolation to satisfy the random channel, and then verifying through tortuosity. There were 36 interpolation schemes dealing with the complex inner wall boundary condition. And the wettability condition was set at the inclinded planes which hydrogen, oil and inner wall contacted. After validating the pf-LBM, we simulated the oil wetting process in the porous media with different catalyst shape under different conditions. According to the numerical results, this work mainly focused on the effect of the catalyst geometry construct, fluid physical properties and operation conditions on the wetting area and efficiency. We studied the laws how the porosity, average pore diameter, tortuosity, catalyst shape, hydrogen/ oil physical properties, hydrogen/ oil ratio and driving force decided the oil distribution. A correlation about the inner wetting efficiency for the catalyst particles was presented. Thus the results are helpful to quantitatively master the inner wetting state and optimize catalyst geometry.

Key words: inner wetting efficiency; phase-field lattice Boltzmann method; geometric construct; porous media; two phase flow

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Applications of shape optimization in complex engineering problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

WRINKLED AND WRINKLE-FREE MEMBRANES

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ABSTRACT

Membranes are easy to buckle and wrinkle due to their extreme flexibilities, leading to the performance degradation and hampering the engineering applications. Here we propose a wrinkle-free approach through optimizing the shape and distribution of interior irregular holes in the membrane. A theoretical model with Marguerre function and complex analysis is performed to accurately estimate the stress distribution and wrinkling capability of the non-uniform membrane. The non-gradient particle swarm optimization (PSO) algorithm is implemented to determine the optimized holes to achieve wrinkle-free performance with ignorable area loss, the computational efficiency has been significantly enhanced through the superposition method. Both post-buckling analyses and physical experiments are carried out to verify wrinkle-free performance of membranes with optimized holes. In addition, an easy-to-implement empirical method is provided to guide the design of wrinkle-free membranes with arbitrary aspect ratio.

MULTI-PHYSICS HIGH-FIDELITY NUMERICAL SIMULATION METHODS FOR METAL ADDITIVE MANUFACTURING PROCESSES

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ABSTRACT

Metal additive manufacturing processes involve multi-physics interaction problems, including heat transfer, fluid dynamics, and solid mechanics. Such complexities challenge conventional numerical methods. This study introduces two novel numerical methods specifically designed to address the multi-physics problems in metal additive manufacturing processes. The first method, called the local multi-mesh finite volume method, efficiently handles heat transfer and melt pool dynamics. It utilizes a dual-mesh system to solve macroscopic temperature across the entire domain and mesoscopic heat and fluid dynamics within the melt pool vicinity. By employing a refinement-by-superposition paradigm, this method enables efficient simulations at the powder scale. The second method, known as the multi-physics material point method, effectively addresses thermo-fluid-solid interactions. It discretizes the material domain using a structured grid and a group of particles for heat transfer, fluid dynamics, and thermal stress solution under both Eulerian and Lagrangian frameworks. This method incorporates a semi-implicit local iteration for phase-changing heat transfer, a modified Chorin's projection method for Darcy's damping, and a staggered derivation scheme for Marangoni forces.

Numerical cases were conducted to validate these methods, and the results were compared with analytical, numerical, and experimental benchmarks. Notably, the local multi-mesh finite volume method demonstrated significantly improved computational efficiency, outperforming the traditional finite volume method by factors of 16 to 50. Furthermore, the multi-physics material point method achieved faster convergence in managing phase transitions, requiring 75% fewer iterations than the traditional bisection and Newton methods. The two methods present promising solutions for addressing the challenges of multi-physics phenomena in metal additive manufacturing.

Data-driven methods for modeling complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A PYTHON TOOLBOX FOR BAYESIAN LEARNING OF PORT-HAMILTONIAN SYSTEMS

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ABSTRACT

Machine learning has emerged as a powerful tool for modeling and control of dynamical systems across various scientific and engineering domains. Dynamical systems, characterized by their evolution over time, can exhibit intricate behaviors that are challenging to capture using first principal methods alone. Hence, utilizing data driven approaches to model complex dynamical systems can offer high accuracy and emerges as a generalizable method. However, for creating robust modeling and safe control of dynamical systems, machine learning approaches has often been hindered by their inherent limitation: a lack of consideration for the underlying physical laws and constraints that govern the behavior of any real-world dynamical system. As a result, the models often lack trustworthiness and generalizability.

In contrast, physics-informed machine learning leverages the inherent knowledge and understanding of the physical world to inform the learning process of machine learning algorithms. By explicitly integrating physical laws, domain expertise, and prior knowledge into the learning framework, physics-informed learning empowers control systems to leverage the flexibility and adaptability of machine learning while remaining grounded in a solid understanding of the underlying dynamics.

In the talk, we will introduce PyGpPhs – an easy-to-use toolbox for physics-informed learning of electromechanical systems. The toolbox is built on our recently introduced Gaussian Process Port-Hamiltonian systems (GP-PHS) which is a physics-constrained, nonparametric Bayesian learning approach with uncertainty quantification. In contrast to many other physics-informed techniques that impose physics by penalty, the proposed data-driven model is physically correct by design. The Bayesian nature of GP-PHS uses collected data to form a distribution over all possible Port-Hamiltonian systems instead of a single point estimate. Thus, the GP-PHS model i) generalizes well, ii) is highly interpretable and iii) the inherent uncertainty quantification enables future safe model-based control approaches. To further demonstrate theory and usages of the toolbox, we will present the learning of the dynamics of a non-harmonic oscillator in detail. The toolbox is easy to use and demonstrate high accuracy in modeling.

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Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHASE FIELD FRACTURE MODEL AND TOPOLOGY OPTIMIZATION FOR ADDITIVE MANUFACTURING

Qing Li[1], Chi Wu[1], Cuiyi Li[2], Jianguang Fang[2] and Grant Steven[1]*

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ABSTRACT

Phase field models have been extensively studied in the analysis of brittle and ductile fracture. However, few have been explored to simulate additively manufactured materials and validated by experimental data so far. This study develops a phase field framework for modelling complex mechanical behaviours of 3D printed metallic and ceramic materials [1]. To consider the 3D printing induced microstructural orientation, transversely isotropic Hill48 and modified Mohr-Coulomb constitutive models are incorporated here to depict the plastic and fracture behaviours, respectively. The numerical results divulge that, by considering the stress state-dependent crack initiation, the proposed phase field model can better simulate the force-displacement responses [1]. Remarkably, the complex fracture sequences, including crack initiation, propagation, and final rupture, can be properly simulated by the proposed phase field model. Importantly, it is necessary to apply a transversely isotropic fracture model to characterise the orientation-dependent fracture behaviour.
Further, the phase-field damage model established is incorporated into the topology optimization framework to consider crack initiation and propagation in a path-dependent fashion [2,3]. The topological design enables to enhance fracture resistance of structures made of additive manufacturing components. A path-dependent shape derivative is developed in a step-wise manner during the nonlinear fracture analysis, which enables to drive the topology optimization properly [3]. To measure the fracture resistance of structure, a p-norm function is formulated to aggregate the phase-field variables into a single constraint. The numerical examples demonstrated that the proposed phase field based topology optimization method can significantly improve the fracture resistance of additively manufactured structures [2]. The proposed method is anticipated to provide an effective approach for sophisticated path-dependent topological design of structures reducing severe stress concentration and high risks of fracture failure.

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Computational mechanics in Canada and China: Current states of shared scientific interests and opportunities for the future cooperation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RECENT PROGRESS IN REACTIVE DIFFUSION MODELLING FOR FLEXIBLE BIOELECTRONIC SYSTEMS

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ABSTRACT

Flexible bioelectronics is a class of technology that involves components which physically disappear, in whole or in part, at prescribed rates and at programmed times. Enabled devices include medical monitors that fully resorb when implanted into the human body (“bio-resorbable”) to avoid long-term adverse effects, or environmental monitors that dissolve when exposed to water (“eco-resorbable”) to eliminate the need for collection and recovery. Theoretical modeling of the behaviors of the constituent materials represents important design tools for flexible bioelectronic systems. In this talk, a class of reactive diffusion models for the analyses and designs of flexible bioelectronic systems are reported, by which the key quantities such as the distribution of water concentration, thickness change, and lifetime predictions are obtained analytically. These models are well validated by the experiments and provide effective approaches to innovative designs of related devices.

Machine learning and multiscale modeling for complex materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT OF VARIATIONAL BAYESIAN LEARNING NEURAL NETWORK FOR SOLUTIONS OF INVERSE PROBLEMS: FROM FORENSIC ANALYSIS OF TRAFFIC ACCIDENTS TO THERMAL DISTORTION CONTROL IN 3D PRINTING

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ABSTRACT

We have developed a class of variational Bayesian learning neural networks-based machine learning algorithms, including a mixed Bayesian variational finite element method, to solve various inverse problems, such as reconstruction of car crash accidents, thermal distortion control in 3D printing, and general structural forensic analysis on fracture and crack propagation. In this work, powerful variational Bayesian learning-based computation algorithms have been developed to “inversely” identify the deformation maps in the sense of continuum mechanics as well as the loading conditions while the only information given is the deformed material shape or geometry.

We developed several novel techniques, such as (1) Variational Bayesian Learning formulation coupled with a Feed-forward architecture, and (2) a mixed Galerkin variational Bayesian learning finite element method and its inverse solution for deformation mappings in any dimension. We have then applied these computational algorithms to several important real engineering applications. We have demonstrated that the developed machine-learning algorithm can practically identify the deformation field of a real crashed car and recover its initial pre-crash state based on residual damaged geometric configuration, and the Bayesian regularization network can provide a powerful geometric deviation control (BRN-GDC) algorithm that has the capability to control the thermal distortion in 3D printing that is parameter- and location-dependent.

In this talk, we present an overview of the theory and computational algorithms of Variational Bayesian learning neural network methods and their applications.

Advanced numerical methods for the modeling and optimization of coupled dynamical systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THERMOELASTIC DAMPING OF FGM MICRO BEAMS BASED ON THE HIGHER-ORDER SHEAR DEFORMATION THEORY

Shirong Li[1] and Zeqing Wan*[1]

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ABSTRACT

Thermoelastic damping (TED) in free vibration of a simply supported functionally graded material (FGM) micro beam with rectangular cross section is investigated based on the classical thermoelasticity. Material properties of the FGM micro beam are assumed to be continuously vary along the beam thickness. Governing equations for the structural vibration coupled with the temperature field are formulated by using Levinson higher-order shear deformation beam theory. Heat conduction equation coupled with the bulk strain is derived on the basis of Fourier model. For small amplitude transverse vibration, we assume that heat conduction effect is dominant in the thickness direction so that the heat conduction equation is simplified as a quasi-one-dimensional differential equation with variable coefficients which are functions of the coordinate in the beam thickness direction due to the transverse inhomogeneity of the materials. A layer-wise homogenization approach is employed to approximately solve the heat conduction equation with variable coefficients, where the FGM beam is divided into numerous uniform layers where the thermal and mechanical properties in each layer are considered to be constant and evaluated at the mid-surface of the divided layer. Consequently, the heat conduction equation possessing variable coefficients is discretized into a series of differential equations with constant coefficients in each layer. Analytical solutions for these equations with the adiabat boundary conditions at the beam top and bottom surfaces and the continuation conditions at the interfaces are obtained in terms of the kinematic quantities. Afterwards, the TED in the FGM Levinson beam is determined by the complex frequency approach in terms of the isothermal frequency of the homogenous Euler-Bernoulli beam by using mathematical similarity between the eigenvalue problems for the two types of beams. Considering an FGM beam with the material properties varying as power functions from full silver (Ag) at the top surface to full silicon (Si) at the bottom one, numerical results are presented to quantitively analyze the effects of the material gradient, the geometry and the shear deformation on the TED and the frequency shift of the micro beams in detail. The numerical results show that the TED evaluated by the Levinson beam theory (LBT) is smaller than that by the Euler-Bernoulli beam theory (EBBT) and the difference becomes significant along with the increase in the value of the thickness-to-length ratio. Therefore, for a thick or moderately thick micro beam the LBT can provide a more accurate prediction for the TED than the EBBT.

Numerical modeling of granular and multiphase flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A DATA-DRIVEN MULTISCALE SURROGATE MODEL FOR CFD–DEM SIMULATIONS

Shuo Li[1] and Mikio Sakai*[1]

[1]*The University of Tokyo*

ABSTRACT

Gas–solid flows are commonly investigated in industries. The CFD–DEM method is an established method for simulating the gas–solid interactions. However, the CFD–DEM simulation of industrial gas–solid flows often requires substantial computational resources. To address this issue, in this study, a novel data-driven multiscale surrogate model, referred to as a reduced-order model coupled with a signed distance function-based graph network (ROM–SGN), is proposed to accelerate the simulation of gas-solid flows. Validation studies are conducted in a fluidized bed. Macroscopic properties such as particle distribution, pressure drop, and bubble distribution are compared between the CFD–DEM and ROM–SGN simulations. The results demonstrate that the ROM–SGN accurately simulates the gas–solid dynamics and significantly reduces calculation time by several orders of magnitude compared to CFD–DEM simulation. This work will contribute significantly to the advancement of simulation and modeling for industrial multiphase flows.

Keywords: CFD–DEM; Surrogate model; ROM–SGN; data-driven coupling.

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Recent advances on interfaces dynamics modeling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A SIMPLE MODEL FOR SIMULATING VESICLE EXPANDING AND SHRINKAGE

Shuwang Li[*1], Steve Wise[2] and Xiaoxia Tang[1]*

[1]*Illinois Institute of Technology*
[2]*University of Tennessee*

ABSTRACT

In this talk, we present a diffuse interface model for vesicle expanding (growth) or shrinkage induced by an osmotic pressure. The model consists of an Allen-Cahn equation describing the evolution of the phase field and a Cahn-Hilliard equation describing the evolution of the concentration field. We establish control conditions for expanding or shrinking vesicles using the concept of common tangent construction in materials science, allowing the exchange of materials between the interior and exterior domains. Numerical experiments reveal that the model can capture the main feature of dynamics: formation of circle-like (expanding) and finger-like (shrinking) vesicles.

Microstructures of chemically complex materials and their impacts on material properties from multiscale simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CURVATURE-CONTROLLED BAND ALIGNMENT TRANSITION IN 1D VAN DER WAALS HETEROSTRUCTURES

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[1]*Westlake University*

ABSTRACT

One-dimensional (1D) van der Waals (vdW) heterostructures of coaxial inorganic nanotubes, such as carbon nanotubes and transition metal dichalcogenide (TMDC) nanotubes, have recently emerged as a new area of endeavor in materials science. A key prerequisite for designing the properties of 1D vdW heterostructures is to understand the band alignment of the coaxial nanotubes in these novel heterostructures. In this talk, I will present our recent first-principles study of the effect of curvature on the electronic structure and band alignment in 1D vdW heterostructures of TMDC nanotubes. We find that, as the diameter of an individual TMDC nanotube decreases, the combined effect of curvature-induced flexoelectricity and circumferential tensile strain causes a rapid lowering of its conduction band minimum, while the valence band maximum exhibits an initial lowering before rising. As individual TMDC nanotubes form coaxial heterostructures, the concerted effect of diameter-dependent band-edge levels and intertube coupling via flexovoltage can lead to a Type II to Type I transition in intertube band alignment in several 1D TMDC heterostructure systems, including large-diameter MoSe2@WS2, MoTe2@MoSe2, and MoTe2@WS2 heterostructures. The results lay down a foundation for the rational design of 1D vdW heterostructures.

Machine learning and data driven based engineering computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BIOMIMETIC CELLULAR MATERIAL UNIT CELL REPRESENTATION AND ON-DEMAND DESIGN BASED ON A TRANSPARENT NEURAL NETWORK AND A NEURAL OPERATOR

Xiang Li[1], Ziming Yan[2], Zhanli Liu[2] and Zhuo Zhuang[2]*

[1]*Hainan Normal University*
[2]*Tsinghua University*

ABSTRACT

Cancellous bone is a natural cellular material that is able to proactively change its microstructure to adapt to the surrounding loading conditions. This adaptability gives the bone anisotropic mechanical properties and the ability to absorb energy. Inspired by the topological and mechanical properties of cancellous bone, this research proposes a framework to represent and design biomimetic cellular materials based on a transparent neural network and a neural operator. In this research, a transparent neural network is used to compute the Gaussian random field and generate the topology of the spinodoid, a biomimetic cellular material. Furthermore, a novel homogenization method accelerated by neural operators is presented to efficiently compute the anisotropic elastic matrices of the spinodoid unit cells, combining improved computational speed with precision. Finally, a data-driven workflow is introduced to inversely determine the topological parameters of the spinodoid unit cell based on the given anisotropic elastic matrix. Numerical examples show that the proposed framework is capable of efficiently and correctly designing spinodoid unit cells with given design goals and can be extended to the design applications of other biomimetic cellular materials.

Recent advances on interfaces dynamics modeling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FRONT TRACKING AND APPLICATION TO PARTACHUTE SIMULATION

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ABSTRACT

We introduce an integrated computational method for the simulation of the parachute system using the front tracking methodology. A dual-stress spring-mass model based on the front tracking method is used to study the dynamics of fabric surfaces in air. The numerical algorithms for this complex physics system includes fabric model and its coupling with the fluid solvers, both incompressible and compressible. The fabric porosity is modeled by the ghost cell method. The collisions, including fabric-fabric, fabric-rigid, rigid-rigid and string collisions with fabric and rigid are implemented. This presentation will introduce on the algorithms and simulation of the
supersonic parachute simulation. We will also present other applications, including fluid interface instabilities, phase transition and particle tracking with the front tracking software library.

Modeling and simulation of dynamics, stability and control of aerospace structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ANALYSIS ON NONLINEAR WHEEL-HOLDING CONTACT ON NOSE LANDING GEAR DYNAMICS CHARACTERISTICS DURING NEW TOWING-OUT MODE OF AIRCRAFT

Xiaoyun Li[*1], Yijun Chai[1], Xiongwei Yang[1] and Yueming Li[1]*

[1]Xi'an Jiaotong University

ABSTRACT

The safety and efficiency of airports are compromised due to civil aircraft commonly using their own engines for taxiing in the current era. A new generation of towing-out mode has been introduced, which utilizes the external power supplied by a towbarless tractor. A complex constraint relationship exists between the nose landing gear's wheel and the wheel-holding mechanism of the tractor during this towing process. The nose landing gear, a crucial component for ground taxiing, possesses dynamic characteristics that directly influence the safety of high-speed taxiing and the service life of the structure. Given the constraint relationship of wheel-holding contact force, it is imperative that a study be conducted on the vibration characteristics of the nose landing gear, which is subjected to both heavy load and towing load. A specific type of civil aircraft front landing gear is selected as the research subject, and a mathematical model is derived to describe the constrain between the nose landing gear's wheel and the wheel-holding mechanism. This derivation is based on the wheel-holding contact geometric relationship and the Winkler contact model. The static and dynamic characteristics of the nose landing gear under heavy load are investigated. Considerations are given to the wheel-holding contact interaction during towbarless towing, the nonlinear axial force of the shock absorber, and the buffering effect of the tractor tire. The influence of wheel-holding contact stiffness and nonlinearity on the vibration characteristics of the structure is also examined. A nonlinear relationship between the radial force and radial deformation of the wheel is revealed by the results, with the degree of nonlinearity inversely proportional to the radius of the clamping rod. As the wheel-holding contact stiffness increases, frequency veering and mode conversion are gradually experienced by the first and second modes of the nose landing gear under full-load towing conditions. The occurrence of frequency steering is observed when a specific nonlinear function relationship is exhibited between the clamping contact force and the stiffness of the tractor tire. Moreover, the nonlinearity of wheel-holding contact stiffness exerts a more pronounced impact on the first-order natural frequency of nose landing gear. The findings of this study can serve as a valuable reference for optimizing the nose landing gear under the new towing-out mode and designing the wheel-holding mechanism.

Numerical methods, mathematical modeling and analysis in material science
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INFER EXPLICIT NUMERICAL SCHEMES FROM IMPLICIT DATA WITH APPLICATIONS TO DEFECT DYNAMICS

Xingjie Li[*1], Fei Lu[2], Molei Tao[3] and Xiaofeng Felix Ye[4]*

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ABSTRACT

Efficient simulation of SDEs is essential in many applications, particularly for ergodic systems that demand efficient simulation of both short-time dynamics and large-time statistics. However, locally Lipschitz SDEs often require special treatments such as implicit schemes with small time-steps to accurately simulate the ergodic measure. We introduce a framework to construct inference-based schemes adaptive to large time-steps (ISALT) from data, achieving a reduction in time by several orders of magnitudes. The key is the statistical learning of an approximation to the infinite-dimensional discrete-time flow map.

We use the classical numerical schemes to derive informed basis functions, leading to a parameter inference problem. We introduce a scalable algorithm to estimate the parameters by least squares, and we prove the convergence of the estimators as data size increases. The numerical tests confirm that ISALT can tolerate time-step magnitudes larger than plain numerical schemes.

Recent advances in computational fracture mechanics and failure analysis
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL SIMULATION METHOD FOR FATIGUE CRACK PROPAGATION IN CLADDED C(T) TEST SPECIMEN

Yanlong Li[*1] and Toshio Nagashima*[1]

[1]*Sophia University*

ABSTRACT

To improve the corrosion resistance and rust prevention properties of nuclear reactor pressure vessel (RPV) in nuclear power plants, stainless steel is welded on the inner surface of vessel as cladding. In such cladded structure, due to the dissimilar material interface, fatigue crack propagation behavior is complex and further researches are required.

In this study, a numerical simulation method based on extended finite element method (XFEM) for fatigue crack propagation in cladded structure is proposed. This method employs 8-node hexahedral continuum elements enriched with only Heaviside step function, which can model planar crack independently of finite elements. For the crack across dissimilar material interface in cladded structure, first, the stress intensity factors along the crack front are evaluated by domain integral method, and then crack front shapes are updated by using Paris' law and then smoothed by the cubic Bezier curves in each region. The crack propagation analysis is performed by repeating this series of processes mentioned above.

In this presentation, fatigue crack propagation analyses for cladded C(T) test specimens are performed. The obtained relationships between crack length and load cycle as well as transition of propagating crack front shapes are compared with those of experiment and validated. It was shown that the proposed method appropriately simulated the fatigue crack growth behaviours in cladded C(T) test specimens.

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NUMERICAL SIMULATION OF THE COMPRESSIBLE STABLE RAYLEIGH-TAYLOR-KELVIN-HELMHOLTZ INSTABILITY WITH DISCRETE BOLTZMANN METHOD

Yaofeng Li[1] and Chuandong Lin*[12]

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ABSTRACT

The Rayleigh-Taylor (RT) and Kelvin-Helmholtz (KH) instabilities are typical fluid instability phenomena that often occur in conjunction. The coupled RTKH system can be categorized as stable or unstable, depending on whether the heavier fluid lies beneath or above the lighter one. In stable RTKH systems, the evolution of physical fields is often accompanied by complex phenomena such as nonlinearity, multiscale effects, and nonequilibrium behavior. These complexities pose challenges for traditional methods. As a mesoscopic method, the discrete Boltzmann method (DBM) is capable of describing both hydrodynamic and thermodynamic behaviors and has recently been applied to study the RTKH instability[1-2]. In this study, we utilize the DBM to investigate the competition mechanism between the suppression and promotion of interface evolution, where stable RT inhibits interface evolution, while KH promotes it. This work aims to enhance our understanding of the nonequilibrium evolution of compressible stable RTKH instability and contribute to the theoretical framework of fluid instability.

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Mechanobiology of cells, vesicles and biomembranes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ANALYZING THE LONG TERM BIOMECHANICAL RESPONSE OF ORTHOKERATOLOGY BY CONSIDERING THE ANISOTROPIC VISCOELASTIC BEHAVIOR OF THE CORNEA

Yifeng Li[*1], Zhuoran Yang[1], Ziming Yan[1], Huibin Shi[1] and Zhanli Liu[1]*

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ABSTRACT

Orthokeratology, an effective myopia correction and control technique widely adopted among adolescents, is increasingly gaining scientific attention. Most existing research focused on analyzing patient corneal morphology data to discern deformation patterns but often fell short in understanding the underlying biomechanical mechanisms. This limitation resulted in the fitting of orthokeratology lenses heavily relying on clinicians' judgment, posing a significant challenge for accurately predicting orthokeratology outcomes, i.e., corneal deformation. This study aims to reveal the mechanisms of orthokeratology by establishing a biomechanical model, facilitating the prediction of corneal deformation. We began by collecting extensive corneal morphological data from clinical myopia patients, based on which we constructed a geometrically personalized finite element model. This model considers the anisotropic, visco-hyperelastic mechanical properties of the cornea. It was validated by simulating the long-term response in central corneal thickness over an 8-day orthokeratology period and comparing these results with experimental data. Furthermore, the study explored the effects of corneal anisotropic characteristics and posterior surface boundary conditions on the shaping process. Corneal shear dominated by indentation was revealed as the key deformation mechanism in orthokeratology. Using this model, we analyzed the effects of lens-wearing time and cycle duration of orthokeratology lenses on myopia correction and proposed appropriate lens-wearing strategies for various degrees of myopia. The biomechanical model established in this research successfully captured the long-term viscoelastic response of central corneal thickness, laying a solid foundation for the quantitative prediction of orthokeratology outcomes.

Machine learning and multiscale modeling for complex materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HIGH-THROUGHPUT SCREENING AND PREDICTION OF HIGH MODULUS OF RESILIENCE POLYMERS USING EXPLAINABLE MACHINE LEARNING

Ying Li[1]*

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ABSTRACT

The ability to store and release elastic strain energy, as well as mechanical strength, are crucial factors in both natural and man-made mechanical systems. The modulus of resilience (R) indicates a material's capacity to absorb and release elastic strain energy, with the yield strength (σy) and Young's modulus (E) as R = σy2/(2E) for linear elastic solids. To improve the R in linear elastic solids, a high σy and low E combination in materials is sought after. However, achieving this combination is a significant challenge as both properties typically increase together. To address this challenge, we propose a computational method to quickly identify polymers with a high modulus of resilience using machine learning (ML) and validate the predictions through high-fidelity molecular dynamics (MD) simulations. Our approach commences by training single-task ML models, multitask ML models, and Evidential Deep Learning models to forecast the mechanical properties of polymers based on experimentally reported values. Utilizing explainable ML models, we were able to determine the critical substructures that significantly impact the mechanical properties of polymers, such as E and σy. This information can be utilized to create and develop new polymers with improved mechanical characteristics. Our single-task and multitask ML models can predict the properties of 12 854 real polymers and 8 million hypothetical polyimides and uncover 10 new real polymers and 10 hypothetical polyimides with exceptional modulus of resilience. The improved modulus of resilience of these novel polymers was validated through MD simulations. Our method efficiently speeds up the discovery of high-performing polymers using ML predictions and MD validation and can be applied to other polymer material discovery challenges, such as polymer membranes, dielectric polymers, and more.

CHARACTERIZING CYCLIC INELASTIC BEHAVIOR OF ANGLE MEMBERS: A MODIFIED HYSTERETIC MODEL

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ABSTRACT

Predicated on the Dicleli physical model [1], a modified hysteretic model tailored for displacement-controlled cyclic loading is devised. Comparative analysis through a finite element model indicates that the interrelation between normalized axial and lateral displacements solely depends on slenderness, ensuring the physical interpretation of the equation's parameters. Additionally, the study also explores the way local buckling alters cross-section shape and macroscopic component behavior. The new model reduces this impact with effective width. Given that the residual lateral displacement of each loading cycle may transform a straight rod into a bow-shaped rod, aggravating second-order effects and triggering early buckling. The improved model integrates geometric nonlinearity by updating the tangent modulus after each cycle, except initial imperfection, which is already included in the derivation of physical model. Since subsequent simulations demonstrate that low cycle fatigue damage and fracture propagation minimally affect the component's hysteresis curve, these factors are excluded from the model. The modified hysteretic model, validated by experimental tests and finite element simulations, effectively captures the key numerical values of the hysteresis curve, enabling a smooth transition from regular to random loading. This study offers a promising methodology for representing the cyclic inelastic behavior of angle members in various structures.

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Multiphysics and data-driven modeling for cardiovascular biomedicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AI-ENABLED RAPID IMAGE-BASED HEMODYNAMIC MODELING AND SIMULATION

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ABSTRACT

Cardiovascular disease (CVD) has persisted as a leading global cause of mortality for decades. While image-assisted computational fluid dynamics (CFD) simulation has proven invaluable in offering comprehensive hemodynamic insights for non-invasive diagnosis and clinical treatment planning for CVD, the conventional approach faces significant challenges hindering its widespread application. Firstly, the manual extraction of geometries from medical images is time-consuming, inconsistent among different operators, and may introduce human artifacts during geometry reconstruction. Secondly, the meshing, case setup, and execution of CFD simulation under realistic settings (e.g., high spatial and temporal resolution, fluid-solid interaction (FSI), Wind-Kessel boundary conditions) can be time-demanding, limiting its applicability in clinical scenarios requiring timely feedback or iterative model queries for device implant design. Thirdly, uncertainties in boundary conditions or model parameters during CFD simulation can compromise result credibility, reducing its effectiveness in clinical diagnosis.

In response to these challenges, we introduce a novel AI-enabled image-based computational modeling framework for automatic patient-specific image segmentation and rapid hemodynamic simulations, which harnesses the potency of deep learning to enable fast prediction of 3D blood flow patterns from raw image scans. Firstly, we automate vessel segmentation in medical imaging by developing a Laplacian-of-Gaussian (LoG) based Bayesian network, enhancing segmentation accuracy across diverse vascular structures. Subsequently, a shape deformation model using graph neural network (GNN) with residual connection reconstructs high-quality patient-specific simulation-ready meshes from segmented voxel images. Surface smoothness on the reconstructed geometry is ensured through the use of a large deformation diffeomorphic metric mapping (LDDMM) method. Finally, a GNN-based CFD surrogate model is established for rapid prediction of simulation results, handling unstructured meshes and featuring full gradient tracking and backpropagation for swift model adjustments and parameter optimization across complex vascular structures. The proposed models are demonstrated on a main aorta with upper branches (brachiocephalic trunk, left common carotid artery, and left subclavian artery), showcasing its merit and effectiveness. This study serves as a compelling indication that the integrated machine learning technologies hold substantial promise and have the potential to revolutionize CVD diagnosis, offering a more effective and efficient tools for cardiovascular healthcare.

Machine learning and multiscale modeling for complex materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTIPHYSICS-INFORMED MACHINE LEARNING FOR ARCHITECTED BATTERY DESIGN

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ABSTRACT

Li-ion batteries (LIBs) are critical for electrification in a wide range of applications to reach zero-net emission goal. These increasingly widespread applications warrant an improvement in the existing battery designs so as to meet this increasing demand. One such possible improvement is the use of Si anode instead of the traditionally used graphite electrode as this change allows for increased battery life, increased capacity, increased safety and better performance. The unique intercalation mechanism of Li ions into the Si anode Si anode results in a better specific capacity of the battery. In this mechanism Si atoms react with lithium, which leads to the bonds between the Si atoms giving way for the formation of the LixSi alloy. However, there is a cost associated with this design improvement. Volumetric changes of upto 300% are observed in the Si anode during the lithiation/delithiation cycles which results in the development of large internal stresses in the anode. Delamination of the Si anode from the current collector substrate and the cracking in the Si anode material itself are the consequences of this volumetric stresses, which causes a reduction in the capacity of the battery. The growth of the solid electrolyte interface (SEI) layer is another capacity fade mechanism that is coupled with mechanically induced damage in the LIBs. SEI layer growth in LIBs can lead to the increase in the internal resistance of the cell and the removal of the active Li material from the cycling process. The growth of the SEI layer on the surface of the anode mainly occur during the battery cycling phase. The continued growth of this layer increases the overall resistance and removes the active Li from the cycling system, thereby reducing the overall capacity of the battery. Hence, to be able to truly utilize Si as the active material for the LIBs, there is a tremendous need to understand these three coupled failure modes in the battery and identify electrode design that can mitigate the mechanically induced capacity degradation. One potential solution is architected electrode. In this study, multiphysics-informed machine learning has been developed to investigate the capacity degradation of architected electrodes with various designs under different operating conditions. This is the first work that can consider all major coupled failure models of Si-based electrodes in the performance analysis, which can facilitate the design of high efficiency battery with architected electrodes.

Fracture, damage and failure mechanics of cementitious materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SYNERGISTIC EFFECTS OF ENVIRONMENTAL DETERIORATION ON FATIGUE AND FLEXURE PROPERTIES OF GLASS FIBER REINFORCED POLYMERIC (GFRP) COMPOSITES : A MULTISCALE AND MULTIPHYSICS MODEL.

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ABSTRACT

This study aims to simulate synergistic UV & moisture deterioration and demonstrate its role in changing the residual fatigue and flexure performance in architectural GFRP composites. This study develops an experimentally validated 3D Multiphysics model at structural level and gets this homogenization-based model to identify each of the degradation mechanisms observed in the experimental data and to analyze the differences that the various degradation mechanisms might make to the properties and durability of the environmental aged composite materials. Sensitivity analyses are conducted to investigate the effect of mesh density on the accuracy of functions homogenized from micromechanical models. The aging-fatigue-bend model with respect to two different deterioration mechanism assumptions is developed and analyzed. Research shows that models with homogeneous damage assumptions allow higher feasibility and convergence when aging concurrently with complicated mechanical loading, while models with surface erosion assumptions describe the actual deterioration mechanism more precisely and offer more freedom, especially when the environmental aging condition is more complicated.

This model can be incorporated into many commercial finite element codes for a sustainability study of composite structures/systems. In future work, the models developed in this study will be combined with life cycle assessment (LCA) tools to support better sustainability-focused new material design, thus reducing costs and environmental impacts in the built environment.

NUMERICAL SIMULATION METHODS AND DATA-DRIVEN MODELS FOR METAL ADDITIVE MANUFACTURING

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ABSTRACT

Metal additive manufacturing (AM) technologies have found the potential to revolutionize the global part manufacturing landscape for their tremendous advantages in building geometrically complex parts with tailorable microstructures and properties. However, they still suffer from unexpected formation defects of the as-built geometry, dimension, and material properties, which require a complete understanding of the process-structure-property relationship. Because the process of metal AM involves extremely multi-physical phenomena taking place at a variety of temporal and spatial scales, high-fidelity numerical simulations are preferred to the costly trial-and-error experiments to address the process-microstructure-property relationship of AM and to aid the process parameters optimization for reducing the final product defects such as surface roughness, void formation, heterogeneous grain structures, etc. In this study, we proposed multi-scale and multi-physics numerical simulation methods, including the proposed multi-physics material point method, extended cellular automaton method, crystal plasticity finite cell self-clustering analysis method, for the powder melting-solidification process, grain structure evolution, and mechanical properties for different as-built alloys with different metal AM processes. The predictions from the proposed computational methods are in good agreement with the experimental data available in the literature for both powder bed fusion and wire-based directed energy deposition processes. Furthermore, data-driven models based on deep learning algorithms for the process-structure-property problems are developed based on the dataset by the proposed numerical simulation methods. The high efficiency and accuracy of these models are demonstrated. It is shown that the proposed methods and models can shed light on the process-microstructure-property relationships and can be further applied to optimizing process parameters.

Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A UNIFIED THEORY FOR SHEAR DEFORMABLE COMPOSITE PLATES

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ABSTRACT

A shear deformation-based unified theory for composite plates is established. The theory contains four unknowns which are explicit to interpret the physical response. Apart from the three common displacement components for a point on the midplane, a remaining higher-order displacement component is exclusively attributed to transverse bending and shear deformation. The transverse shear deformation of the function distribution can be represented by general shape functions. The elucidation of the thickness locking mechanism relies on the innovative displacement component introduced in this study, which improves the kinematic assumptions inherent in conventional plate/shell theories. Further, the present theory explicates the explicit physical terms associated with transverse normal stress and strain. In addition, the present unified theoretical framework, along with the corresponding assumptions, induces further simplification and transition into the conventional plate theories, namely, first-order shear deformation theory (FSDT), higher-order shear deformation theory (HSDT), and others. Exact analytical solutions of composite plates are obtained. A comprehensive numerical investigation has been performed, encompassing diverse plate theories and various composite structures, including functionally graded material (FGM) plate structures, FGM sandwich plate structures, etc. The clarity and unity in the present theory and the physical meanings can be elaborated by integrating the conventional theories under certain assumptions.

Recent advances in high-order methods for computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SPECTRAL DIFFERENCE SOLUTIONS OF TWO THREE-DIMENSIONAL KINEMATIC DYNAMO PROBLEMS

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ABSTRACT

We report a recent development of the high-order spectral difference method with divergence cleaning (SDDC) for accurate simulations of two 3D kinematic dynamo benchmark problems on unstructured grids consisting of high-order iso-parametric hexahedral elements. The divergence cleaning approach is based on the improved generalized Lagrange multiplier (GLM), which is thermodynamically consistent and Galilean invariant. The Spectral Difference with Divergence Cleaning (SDDC) method has been used to successfully model a number of nonlinear MHD problems. The spectral difference method is a versatile high order method that can be used for unstructured grids and can be massively parallelized. The first kinematic dynamo problem was solved in a cubic box with all periodic boundary conditions. The SDDC method will be verified to capture the “Cigar” structures published in the literature. The second kinematic dynamo problem adopts a spherical shell geometry and non-penetrative and stress-free boundary conditions. The SDDC method will be employed to predict Sunspot cycles.

Buckling analysis and design of thin-walled structures based on novel and intelligent computational methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A REDUCED-ORDER METHOD WITH MIXED NONLINEAR KINEMATICS FOR GEOMETRICALLY NONLINEAR AND BUCKLING ANALYSIS OF THIN-WALLED STRUCTURES

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ABSTRACT

Thin-walled structures subjected to the in-plane and out-of-plane loads are widely used as load-bearing components in the aircraft, space and various civil engineering fields. The out-of-plane deflection of thin-walled structures is normally much larger than the wall thickness when the external load is applied laterally and/or buckling occurs. In these cases, a geometrically nonlinear analysis is required to achieve a realistic load-displacement response which greatly influences the load-carrying capability of thin-walled structures.

The conventional finite element (FE) method with a Newton-Raphson incremental-iterative technique still has limitations for geometrically nonlinear analysis. The repeated linear solutions of a large full-order FE system are computationally expensive, limiting the step size of the path-following analysis. In addition, a sufficient number of path-following steps must be adopted to achieve a geometrically nonlinear response curve with a favorable smoothness. This further aggravates the computational burden of geometrically nonlinear analysis.

In this work, a novel reduced-order method in the framework of mixed nonlinear kinematics is proposed for the geometrically nonlinear analysis of thin-walled structures with large deflections and/or buckling. The mixed nonlinear kinematics are developed in the combination of co-rotational and updated von Kármán formulations. The co-rotational kinematics are used to calculate the internal force and tangent stiffness of the structure, whereas the third- and fourth-order strain energy derivatives are achieved using the updated von Kármán kinematics. For the geometrically nonlinear problem with large deflection, reduced-order models with one degree of freedom are constructed based on the perturbation theory, otherwise more degrees of freedom are involved in the presence of buckling. The use of mixed nonlinear kinematics can greatly improve the computational efficiency in construction of a reduced-order model. The solutions of reduced-order models can be regarded as nonlinear predictors to the geometrically nonlinear response. Nonlinear predictors are required to be corrected using internal force-based residuals to ensure the accuracy of the geometrically nonlinear analysis. A geometrically nonlinear response with favorable smoothness is efficiently and accurately achieved using large step sizes in the path-following analysis. Various numerical examples are applied to validate the numerical accuracy and efficiency of the proposed method.

HINGE AND SMOOTHED-HINGE MODELS FOR CLOTH SIMULATION

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ABSTRACT

The hinge model commonly used in fabric and cloth simulation quantifies bending energy in terms of the angle between the triangular facets defined by four computational nodes with translational but not rotational dofs. The classical hinge model (CHM) starts with the angle between two vectors normal to the triangular facets and derives the first and second order derivatives of the angle for the subsequently nonlinear solution process. In this study, an alternate but an equivalent angle or hinge angle is employed. It leads to the same set of derivatives, but the derivation process appears to be simpler. The torsional stiffness of the hinge is often calculated from the bending energy in one-third or the total area of the two triangular facets which are assumed to be under the cylindrical bending curvature fitting the hinge and the two computational nodes away from the hinge. In this submission, a smoothed-hinge model (SHM) is proposed in which a smooth cylindrical surface is first defined by interpolation at the four computational nodes of the hinge. Under the small curvature and small strain assumptions, the curvatures along the perpendicular directions to the three edges of a triangular facet can be expressed as linear functions of the nodal displacement. The three normal curvatures are transformed into the three curvature components defined in two orthogonal axes on the tangential plane of plate/shell and the conventional bending stiffness matrix used in the plate/shell is used to compute the bending energy. By incorporating the corotational concept, the bending energy can be approximated as a quadratic function of the nodal displacement. As a result, the Hessian of the bending energy is a constant matrix and does not require to be updated in the iterative solution procedure. For the membrane energy, a six-node interpolation instead of the three-node interpolation is employed. The former, when combined with either CHM or SHM, effectively mitigates the occurrence of sharp crease artifacts. To model contact and friction conditions, the incremental potential contact (IPC) is employed. Quasi-static and elasto-dynamic problems are both examined. Through quantitative and qualitative numerical experiments, the results demonstrate that our computational models exhibit stability with large time steps and convincingly simulate a variety of draping and garment scenarios.

Modeling friction and wear
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A GENERAL CONTACT MODEL FOR ROUGH SURFACES BASED ON THE INCREMENTAL CONCEPT

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ABSTRACT

It is now widely accepted that the real contact area between rough solids rises linearly with increasing normal loads. However, the coefficient of proportionality varies among different theoretical models and simulation results. This study advances a model for analyzing the elastic contact of rough solids. By taking into account the specific shape of contacting asperities, the connection between the real contact area and geometric truncation area is established in priority. Furthermore, the relationship between geometric truncation area and normal load is addressed by adopting the incremental concept. For surfaces covered with spherical asperities, the model could reproduce the predictions provided by the celebrated GW model [Greenwood, J. A., and Williamson, J. B. P., 1966, Proc. Roy. Soc. A., 295(1442), 300-319]. Avoiding prescribing the asperity geometries, the model tends to be more robust when surfaces are random and fractal. For general fractal Gaussian random rough surfaces, the model suggests that the coefficient of proportionality lies between 1.67 and 2.56. The upper and lower limits are close to the predictions of the BGT model [Bush, A. W., Gibson, R. D., and Thomas, T. R., 1975, Wear, 35(1), 87-111] and Persson's theory [Persson, B. N. J., 2001, J. Chem. Phys., 115(8), 3840-3861], respectively. In the thermodynamic limit, the potential varying scope for the coefficient of proportionality is further narrowed ranging from 1.92 to 2.22. The resultant predictions are in accord with numerical results presented in literature. The current study might provide profound insights into understanding the role of surface morphologies in elastic rough contact.

Advanced techniques for transport phenomena in heterogenous porous media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL SIMULATION INVESTIGATION ON NONLINEAR FLOW CHARACTERISTICS OF ROUGH SINGLE FRACTURES WITH DIFFERENT CONTACT AREAS

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ABSTRACT

Abstract: To comprehensively understand the influence of the contact area on the flow characteristics of rough single fractures, a rough fracture surface is initially constructed using a spatial frequency domain approach. Subsequently, rough single fractures with varying contact ratios are derived by translating and displacing the fracture surface. The Navier-Stokes equation and Mass-conservation equation are solved by utilizing the laminar flow module integrated within the COMSOL software. The simulation results show that the nonlinear correlation between fluid flow velocity and pressure gradient can be described by using Forchheimer equation. Under the same flow velocity, a higher contact rate will exacerbate the nonlinear characteristics of fluid flow. In contrast to non-contact fractures, the streamlines within contact fractures exhibit increased tortuosity, accompanied by an elongation of flow pathways. Furthermore, with an expanding contact area, the complexity of the streamline pattern amplifies. The overall pressure field distinctly exhibits non-uniform characteristics, with larger pressure gradient observed within localized contact regions, consequently facilitating an increase in flow velocity.

Keywords: Rough fractures; Contact area; Nonlinear flow characteristics; Numerical simulation.

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MULTISCALE MODEL REDUCTION FOR INVERSE HEAT CONDUCTION IN HIGH-CONTRAST MULTISCALE MEDIA

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ABSTRACT

Efficient numerical simulations for forward problems are crucial for decision-making applications like inverse problems and optimal design. However, when dealing with multiscale medium properties, direct numerical simulation of the forward problem becomes computationally expensive, requiring a fine grid to capture variations in highly oscillating material properties. To address this, model reduction techniques are necessary. In this presentation, we introduce a novel multiscale model reduction method for inverse heat conduction in high-contrast multiscale media, significant in various engineering and industrial applications. Our method, grounded in recent advances in multiscale finite element methods, computes multiple localized multiscale basis functions per coarse region using local spectral problems and the localized energy minimization principle. We provide a theoretical analysis of the proposed method and present several numerical tests to verify its performance.

THE EXTENDED MATERIAL POINT METHOD FOR MODELLING EVOLUTION AND INTERACTION OF MULTIPLE DISCONTINUITIES

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ABSTRACT

The Extended Material Point Method (XMPM) has demonstrated efficacy in numerically simulating shear band evolution and post-failure behavior during large deformations. However, the current formulation of XMPM is inherently limited to representing a single discontinuity, constraining its application in modeling intricate scenarios involving multiple discontinuities. This paper introduces a comprehensive extension to the XMPM framework to overcome this limitation, enabling the simulation of realistic problems characterized by the presence of multiple discontinuities.

Our enhanced method incorporates modifications to the original particle displacement approximation, empowering the XMPM to effectively handle multiple discontinuities within the material domain. Additionally, a dedicated contact strategy is developed to deal with the interaction between these multiple discontinuities within the XMPM framework. Several numerical case studies demonstrate the proposed extension's efficacy in simulating scenarios with multiple discontinuities, which is expected to contribute significantly to the understanding and prediction of material failure in various engineering and scientific applications.

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Certification of simulations and model adaptation in computational science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADAPTIVE GRID REFINEMENT FOR HIGH-ORDER FINITE VOLUME SIMULATIONS OF UNSTEADY COMPRESSIBLE AND TURBULENT FLOWS

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ABSTRACT

This study investigates dynamic mesh adaptation (DMA) for hybrid RANS/LES (HRLES) simulations of compressible turbulent flow. HRLES models, which blend Reynolds-Averaged Navier-Stokes (RANS) and Large Eddy Simulation (LES), are by their nature very sensitive to the computational mesh, because of the very different resolution requirements in the RANS and LES regions. The proposed DMA strategy relies on a high-order k-exact finite volume spatial discretization [1] designed to ensure robust, accurate and conservative solutions for compressible flows with strong discontinuities while limiting the numerical dissipation of vortical structures. A mesh refinement criterion related to the truncation error of the k-exact reconstruction scheme is introduced, and compared with several heuristic refinement criteria from the literature [2]. To limit the computational burden of frequent re-meshing for unsteady flow simulations, the adaptation is performed only at certain time steps, and the error criterion is averaged over the chosen adaptation period [3]. A simple and effective criterion is then introduced to automatically control the averaging and adaptation period. The proposed DMA strategy is evaluated against a series of test cases of increasing complexity, ranging from inviscid vortex advection to turbulent transonic flow past an axisymmetric backward-facing step, representative of the base flow behind a space launcher.

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Emerging topology and shape optimization techniques in computational design of materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ANALYTICAL DESIGN SENSITIVITY INFORMATION OF COMPOSITE LAMINATE SHELLS

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ABSTRACT

Fiber-reinforced composites represent a class of materials celebrated for their exceptional strength, lightweight nature, and versatility. These advanced materials are composed of a matrix, often a polymer, reinforced with fibers such as glass, carbon, or aramid. The strategic integration of these fibers provides unique mechanical properties to the composite, combining the high strength of the reinforcing fibers with the flexibility and formability of the matrix material. This synergy results in materials that are widely employed across various industries, ranging from aerospace and automotive engineering to construction and sports equipment manufacturing. The tailored design possibilities and superior performance characteristics of fiber-reinforced composites make them a focal point of research and innovation in materials science and engineering.

In the optimization of laminated composite shells, diverse objective functions are sought depending on the intended use of the structure. This also applies to the selection of design parameters, where, in some cases, alterations in fiber orientations are desired without affecting the thickness of the structure, while in other instances, only specific layer thicknesses, and possibly their fiber orientations, may be subject to variation. This study explores fundamental types of design parameters for composite laminates, including total thickness, specific layer thicknesses, and fiber orientations, with the derivation of sensitivity relations.

Based on the solid shell formulation described in [1], investigations have been conducted for the extension to anisotropic material behavior, cf. [2], and exploring sensitivity relations concerning the shell geometry, cf. [3]. In this work, these methodologies have been used to formulate efficient sensitivity relations of composite shell structures. Employing a variational approach that embeds sensitivity analysis into the continuum mechanical framework, sensitivity relations for layer thicknesses and fiber orientations are established. These continuously derived quantities can be readily discretized and incorporated into a finite element environment.

Numerical examples are referenced to discuss various aspects, such as computational performance, numerical accuracy, and algorithmic treatment.

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A HYBRID VIRTUAL ELEMENT FORMULATION FOR PLANE ELASTICITY

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ABSTRACT

The enhanced Virtual Element Method (VEM) formulation, recently proposed by D'Altri et al. [1] for plane elasticity, provides numerous advantages over the classic VEM. The main innovation resides in the expression of the projection condition through an energy norm in which a divergence-free interpolation is assumed. This leads to the absence of stabilisation terms and a considerable accuracy improvement.
This work shows how the minimisation of Total Potential Energy and the projection operation typical of enhanced VEM can be obtained from the stationarity condition of the Hellinger-Reissner mixed functional. Starting from this theoretical result, a family of polygonal elements for plane elasticity is proposed, named as Hybrid Virtual Element Method (HVEM). The primary unknowns are the displacements along the element contour, as usual in classic VEM, and the stress field. The latter is assumed to within a polynomial basis that a-priori satisfies the equilibrium equations expressed on a Cartesian frame and corresponds to the divergence-free assumption in the projector term in enhanced VEM formulations. Then, all the discrete operators can be evaluated through line integrals, facilitating the formulation for polygonal elements with a generic number of edges [2].
The HVEM not only provides a wider theoretical background, but also reveals a close relationship with mixed hybrid-stress Finite Elements (FEs) [3], traditionally limited to triangular or quadrilateral geometries. Then, leveraging the broad literature on the hybrid-stress FEs behaviour, we discuss the critical role of selecting appropriate stress interpolation functions, not only for the element stability, but also for the accuracy improvement. In particular, a so-called iso-stable interpolation, that adopts the minimum number of stress parameters to ensure the element stability, turns out to be the optimal choice for achieving accurate solutions also for coarse meshes.

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INVESTIGATING EVOLUTION OF VOIDS IN AL2219 USING 3D CHARACTERIZATION AND CRYSTAL PLASTICITY SIMULATIONS

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ABSTRACT

In this work, emerging high-resolution computed tomography (CT) and crystal plasticity (CP) simulations are used to understand void growth mechanisms in aluminum alloy 2219. By combining experimental and computational results, we investigate how microstructural features such as grain boundaries, triple junctions and particles influence void growth. Both DCT (Diffraction Contrasted tomography) and XCT (X-ray Computed Tomography) techniques are used to characterize initial crystal orientations, voids and phases, and their evolution at various applied strains. On the modeling side, high-fidelity crystal plasticity simulations are performed at the same resolution as CT measurements to obtain local stress/strain fields, stress triaxiality and Lode parameter that are frequently used to understand the void growth. Developed framework enables direct and quantitative comparisons between experimental and computational results for understanding void growth mechanisms in metal alloys.

IDENTIFYING CRACKED/DAMAGED STRUCTURES AND THEIR LOCATIONS USING PHYSICS-INFORMED MACHINE LEARNING WITH SPARSE MEASUREMENTS

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ABSTRACT

In this paper, we introduce a novel method for identifying cracked or damaged structures and precisely locating these flaws by integrating physics-informed machine-learning techniques. Our approach combines principles from physics with advanced machine learning algorithms to address longstanding challenges in structural damage detection. By analyzing the vibrational, acoustic, and quasi-static properties of structures, we extract valuable insights from sparse measurement data to detect subtle indicators of structural degradation. Through rigorous experimentation, we validate the effectiveness and precision of our method in detecting structural damage, highlighting its potential to revolutionize current practices in structural health monitoring and maintenance. To demonstrate the performance of the proposed work, several practical examples, such as cracked and damaged structures, were treated. Finally, it was found that the proposed approach is sufficiently accurate despite a few sensor measurement data. It means that it has great potential to evaluate the anomaly detection of large engineering structures.

Mathematics and algorithms for predictive digital twins (DT)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HYBRID SURROGATE MODELING FRAMEWORK AND REINFORCEMENT LEARNING FOR DIGITAL TWIN APPLICATIONS

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ABSTRACT

Nuclear energy has high operational risks that a digital twin (DT) can aid in the areas of operations & management (O&M); reactor safety analysis and improvement of plant efficiency. A system surrogate model is developed to predict physical asset quantities (e.g. reactor, heat exchanger, pumps) and computational assets responses (e.g. control system). The system surrogate model is labeled hybrid because it leverages the accuracy of physical models for robustness while also integrating low-fidelity models for speed and predictive capabilities. The framework is applied to a Pebble-Bed Fluoride-Salt-Cooled Reactor (PB-FHR), a new-generation reactor that has drawn interest from both research institutes and commercial companies. The physics-based models are used to compute the relative xenon concentrations and pump degradation, both essential quantities that determine the current reactor conditions. The remaining quantities are predicted using a Vector Autoregressive Moving Average with Exogenous term (VARMAX) model trained with data generated from the System Analysis Module (SAM); a transient system analysis tool for advanced reactor concepts. This model can also update itself by assimilating online measurements. The system state awareness provided by the surrogate model is utilized for the reinforcement learning (RL) of weighing plant operations, predictive maintenance and market performance.

New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION IN MAGNETIC FIELD USING HIGH-FREQUENCY HOMOGENIZATION METHOD

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ABSTRACT

Since the driving performance of a magneto-mechanical system is dominated by the magnetic flux distribution, optimizing the shape of the ferromagnetic material (FM), which determines the path and intensity of the magnetic flux, is the most important design process for improving system performance. The important properties of FMs considered here are the magnetic permeability, which describes the amount of magnetic flux generated due to the magnetic field intensity, as well as the energy loss characteristics due to magnetic hysteresis and eddy currents. In particular, since most magneto-mechanical systems currently under development for industrial devices use alternating electric fields, energy loss occurring within FMs is a critical factor that increases the operating temperature of the system and impairs performances. Therefore, in order to design a high-performance system, it is necessary to use a FM that simultaneously satisfies high permeability, low hysteresis, and low eddy current loss, however it is difficult to develop a new material with these properties.
This study aims to optimize both the microstructure of the FM composite and the shape of the magnetic core using the topology optimization method with a large degree of design freedom [1], and apply the optimized magnetic core with high magnetic permeability and low loss coefficient to a magnetic actuator. To do this, a high-frequency homogenization method, which uses a complex permeability tensor to consider the frequency of the applied magnetic field and predict the eddy current loss density of FMs [2], is applied to magnetic field analysis and design. The optimization problem is formulated to optimize the element density and orientation of the core for achieving the target force and flux distribution, while optimizing the microstructure of the FM that can reduce loss even at high frequency of the applied magnetic field. To verify the effectiveness of the proposed design method, optimized results of a linear oscillatory actuator with high operating frequency are introduced.

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Computational models and methods for predicting cancer progression and treatment response
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PATIENT-SPECIFIC OPTIMIZATION OF THERAPEUTIC REGIMENS VIA DIGITAL TWINS TO IMPROVE TRIPLE NEGATIVE BREAST CANCER RESPONSE TO NEOADJUVANT THERAPY

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ABSTRACT

Neoadjuvant therapy (NAT) is the standard of care for locally advanced triple-negative breast cancer (TNBC). However, pathological complete response (pCR) rate in TNBC patients to current NAT regimens is 50-60% [1]. Aside from the need to develop new therapies with higher efficacy and lower toxicity, a critical barrier to improving TNBC response is the lack of rigorous ways to personally tailor therapeutic regimens. We seek to address this challenge by employing digital twins (i.e., mathematical models that provide a virtual representation of individual patients to predict changes in tumor status) to systematically evaluate TNBC patient's response to different NAT regimens, thereby patient-specifically optimizing treatments.

A cohort of TNBC patients (n = 37) from the ARTEMIS trial (NCT02276433) [2] was used for this study. For each patient, standard-of-care NAT chemotherapy was administered (i.e., 4 cycles of Adriamycin/Cytoxan (A/C) every 2-3 weeks, followed by 12 cycles of weekly Taxol (T)) and longitudinal MRIs were collected before and during NAT. Post-surgical pathology was performed to assess final response status. A digital twin framework has been developed by integrating longitudinal MRIs with a mechanism-based model to predict the treatment response [3]. The model was based on a reaction-diffusion equation that describes the change in tumor cellularity due to migration, proliferation, and drug-induced death. With parameters personalized using the MRIs, the patient-specific model (i.e., digital twin) was used to estimate individual patient's response to 128 simulated but clinically feasible schedules of A/C/T. The predicted response (pCR or non-pCR) from each alternative schedule was compared to the patient response from their actual treatment to evaluate the effect of altering treatment regimens.

We observed that, without changing the total dose, shortening the duration of A/C/T administration increased the treatment efficacy. The effectiveness of altering the schedules varied substantially in different patients. In particular, 8 out of 18 patients who had non-pCR responses to their actual treatment were predicted to achieve pCR with the dense-dose Taxol (i.e., 4 cycles of biweekly Taxol), indicating a 21.62% improvement of pCR rate in the study cohort. We are currently applying the optimization to a larger cohort (n > 130).

The preliminary results of our approach provided a unique opportunity of improving TNBC response to NAT through patient-specific optimization of therapeutic schedules. Ongoing efforts focus on accounting for toxicity and investigating the effects of altering therapy type, dose, and schedule on patient response.

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Computational fluid dynamics (CFD) and fluid-structure interaction (CFSI): Methods and Applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A SIMPLIFIED FLUID STRUCTURE ANALYSIS OF AN ELASTOMERIC SINGLE-LOBE PROGRESSIVE CAVITY PUMP

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ABSTRACT

Widely used in the petroleum industry, progressive/progressing cavity pumps (PCPs) were conceived by René Moineau in the 30s and are in continuous design and efficiency improvement. Notwithstanding, PCPs with an elastomeric stator suffer an efficiency decrease due to elastic deformation provided by the fluid pressure rise along the rotor: in cases with interference, the pressure can cause a clearance, and in cases with clearance, the gap expands. To simulate this phenomenon, the present work improves the model proposed by [1] for the analysis of two-way fluid-structure interaction (FSI) in PCPs, by coupling the element-based finite volume method (EbFVM) for the fluid flow field with more general analytical models for the structural deformation field. The previous simplified structural model was implemented as a FORTRAN subroutine accounting for the local fluid pressure as the structural load in a Hookean linear model for radial deformations only [1]. Although the proposed model can still be considered simplified, it extends the previous one-dimensional structural model to a linear plane stress state considering the Poisson effect, thus making it more realistic. The main goal is to establish a reliable procedure for the development of a three-dimensional structural model for analysis of two-way FSI in PCPs that does not require expensive computational costs, as it is currently required in this type of analysis. The EbFVM was implemented in ANSYS/CFX with a developed FORTRAN code (a DLL routine) for structured mesh generation for each time step analysis accounting for the PCP rotor/stator relative motion [1,2,3]. The results were compared with those obtained with the ANSYS/CFX native mesh deformation algorithm, and with those obtained with the previous one-dimensional approach, showing better accuracy, since the first method causes mesh distortions and hysteresis, whereas the second method does not capture the deformations developed in the angular directions of the stator cross-section.

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Advances in computational biomechanics and mechanobiology
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN EFFICIENT SEMI-ANALYTICAL APPROACH FOR THE STOCHASTIC ANALYSIS OF SOFT BIOLOGICAL STRUCTURES

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ABSTRACT

Introduction: Integration of variability and stochasticity in predictive finite element models of biological systems is of critical importance, particularly in the context of diverse populations, whereby, besides intra-individual variability, there are statistically significant differences in biophysical and microstructural properties across ancestry and age groups. In a mechanobiological context other sources of variability include boundary and loading conditions as well as biochemical factors and their driving forces [1]. Stochastic finite element (SFE) analyses aim to propagate stochastic properties of a system directly through the governing partial differential equations but are more complex to implement and computationally expensive than their deterministic counterparts [2]. It is therefore advantageous to develop general and efficient methodologies to conduct such analyses, especially those that can capture spatial variations of random variables (i.e. stochastic fields).

Method: Here, it is proposed to represent stochastic fields using the Karhunen-Loève (KL) decomposition and calculate the stochastic response of the system using a second-order sensitivity analysis [2, 3]. The numerical implementation, based on automatic differentiation, is general and modular, valid for arbitrary kinematics and constitutive laws, making it particularly attractive to model biological soft tissues and their inherent heterogeneities. KL decomposition is computed via the formulation of a macro-element associated with a Fredholm integral equation of the second kind involving the covariance kernel of the stochastic field, and whose solution is obtained via standard Galerkin procedure.

Results: The SFE framework was assessed on various examples by accounting for geometric and material stochastic fields on 2D geometries, and solutions compared to Monte-Carlo simulations. A path-following method was used to solve the geometrically and materially non-linear problems. The gain in computational speed afforded by the semi-analytical approach could reach four orders of magnitude.

Discussion and Conclusion: The ability of a perturbation approach to capture propagation of uncertainties in highly non-linear systems is inherently limited by the expansion order (here, second order). However, the use of automatic differentiation combined with optimisation of computer code means that extension of the SFE framework to higher orders is possible and should be explored in the future. The numerical framework presented here provides an attractive platform to rapidly and statistically explore the influence of multiple factors on the physics of biological tissues and structures.

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Modeling and simulation of the electro-chemo-thermo-mechanical interactions in energy transition and energy storage systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

QUANTITATIVE NUMERICAL STUDIES OF LITHIUM ELECTROPLATING: VISCOPLASTIC INFILTRATION AND CRACKING IN A SOLID ELECTROLYTE

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ABSTRACT

This talk proposes a mechano–electrochemical multi-phase field (MPF) model to study electroplating in ASSLB, which induces cracking and short–circuiting. Different from previous models [1 - 4], in this model, large viscoplastic deformation is involved to account for huge eigenstrain induced by electroplating; The plating reaction is described by generalized BV equation involving Eshelby stress tensor, which introduces effects of conformational volume change and deformation energy on overpotential; Contact between solid phases is considered to simulate different modes of Li growth associated with mechanical constraint; MPF framework incorporated fracture–PF model to describe cracking and viscoplastic infiltration of Li. Accuracy of proposed model is validated by quantitatively comparing simulated and experimental findings [5].

This model provides a comprehensive depiction of the transition from vertical elongation to shank–expansion of Li whisker for low–voltage plating scenario with variable constraints. It indicates a transition from reaction–controlled root–growth of Li whisker to viscoplastic flow of Li in gaps or cracks. Critical time for transition, depending on bias voltage and stack pressure is quantitatively predicted.

In high–voltage plating with rigid constraints, simulation shows that cracking is caused by wedge-opening mechanism. Specially, if LLZO particle is tightly constrained, Li can only fill in narrow crack via viscoplastic flow rather than pushing sidewalls apart to increase deposition space, quickly resulting in a short circuit. If the LLZO particle is not constrained, the growth of Li changes from the fissure eruption to root–growth that widens the crack and considerably extends short–circuit time. It indicates that reducing mechanical constraints of electrolyte particles instead of increasing their mechanical strength or decreasing defect size can improve cyclability of solid–state battery or mitigate short–circuit.

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Advance and application of meshfree methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INTEGRATING DEEP ENERGY METHODS IN THERMOELASTICITY AND PIEZOELECTRICITY

Kuan-Chung Lin[*1], Kuo-Chou Wang[1] and Cheng-Hung Hu[1]*

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ABSTRACT

This comprehensive study combines two pioneering research works that investigate the use of the deep energy technique for difficult multi-physics issues, especially in thermoelasticity and piezoelectricity. The deep energy approach, which is well-known for its resilience in dealing with nonlinearities and producing exact findings, has been intensively investigated for its efficiency and accuracy in these sectors. The first section of the research looks at its use in thermoelasticity [1], examining how network parameters such as layers, neurons, and activation functions affect result accuracy. Successfully resolving 1D and 2D thermoelasticity issues, which compare favorably with analytical solutions and empirical data, has confirmed this technique. The second portion applies this concept to piezoelectricity [2], solving complex 2D piezoelectric issues as well as piezoelectric composite plate actuators. The tanh activation function emerges as a really useful tool, considerably improving accuracy. This two-part study not only proves that the deep energy method can be used instead of traditional numerical methods to solve multi-physics problems, but it also shows how to set up neural networks in the best way to make them work better and more accurately. This will help both computational physics and engineering.

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Recent advances on interfaces dynamics modeling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STABILITY AND ERROR ANALYSIS OF GENERALISED SAV SCHEMES FOR A DIFFUSE-INTERFACE TUMOUR GROWTH MODEL

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ABSTRACT

In this talk we consider a diffuse-interface (phase-field) model for tumour growth that takes into account nutrient consumption and chemotaxis. The model is described by a nonlinear system consisting of a Cahn-Hilliard-type equation coupled with a reaction-diffusion equation. We first prove the existence of its weak solutions. Efficient schemes are then constructed based on the idea of scalar auxiliary variable (SAV), which we show are not only decoupled and easy to implement, but also have the properties of mass conservation and unconditional energy stability. Furthermore, we derive rigorous error estimates of one of the schemes. Several numerical examples are presented to validate the accuracy and stability of the proposed schemes. It is worth noting that when the scheme is equipped with an adaptive time-stepping strategy, it effciently simulates the typical phenomena of aggregation of multiple tumours with different shapes and tumour chemotactic growth. This is a joint work with Zhaoyang Wang and Junxiang Yang.

Uncertainty quantification and reliability analysis in engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PROBABILISTIC INDOOR NAVIGATION AND OBJECT MANIPULATION OF AUTONOMOUS MOBILE ROBOTS

Po Ting Lin[*1], Shaneza Fatma Rahmadhanty[1], Yu-Chun Huang[1], Ikjin Lee[2] and Kuei-Yuan Chan[3]*

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ABSTRACT

Recently, Autonomous Mobile Robots (AMRs) have become promising solutions for the tasks of picking, transporting and placing objects within dynamic environments in smart factories. AMRs are required to position and navigate themselves within an indoor space that is filled with stationary obstacles such as walls, shelves, tables, machines, etc. as well as moving personnel. Ensuring high precision in the positions and configurations of AMRs is difficult due to factors such as wheel slippage, mechanical part backlash, unstable vibrations, sensor inaccuracies and environmental changes. In this paper, the uncertain motions of a 9-degree-of-freedom AMR (i.e., 3 for the ground vehicle and 6 for the robot arm) have been studied and a probabilistic approach for path and motion planning of AMR has been proposed. The probability that the shortest distance between the AMR and the nearby obstacles exceeds the allowable limit was consistently kept at a safe level. In the optimization process of AMR path and motion planning with obstacle avoidance, a linear probabilistic constraint with respect to the AMR control parameters was utilized to maintain the desired reliability level. In this approach, a Most Probable Target Point (MPTP) was found at the tail of the random distribution of the AMR configuration, which has a shortest distance to a Most Probable Failure Point (MPFP) on the nearby obstacle. Both MPTP and MPFP, which were simultaneously determined by a sub-optimization process, were essential for the formulation of the linear probabilistic constraint. Various numerical examples were utilized to show the performance of the proposed Probabilistic Indoor Navigation and Object Manipulation (PINOM) of AMR.

Multi-scale and machine learning-based modeling methods for optimization and design of composites
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A FAST PREDICTION METHOD FOR BEARING STRENGTH OF AIRCRAFT COMPOSITE BOLTED STRUCTURES CONSIDERING INITIAL ASSEMBLY DEVIATION

Qingyuan Lin[*1], Yong Zhao[1], Yuming Liu[1], Wei Pan[1], Wencai Yu[1] and Yu Ren[1]*

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ABSTRACT

The application of advanced composite materials is currently a key approach to improving the performance of high-end equipment such as aerospace. Joints are the weak points of composite structures. More than 60% of the failure of composite structures occurs in the connection position. Mechanical behavior analysis and joint performance prediction of the assembly and loading process of the composite structure is the key guarantee to realize its expected performance. Bolted joins are the most important form of assembly for composite structures. In the assembly process of composite bolted structures such as airplane wings, due to the influence of the complex multi-source uncertainty factors such as the manufacturing errors of the parts, the accumulation of errors in the pre-procedure assembly process, and the deviation of the assembly tooling, composite laminates always have initial assembly deviations, which are mainly manifested in the shape deviation of the parts and the relative position deviation between the parts. The above shape-position deviations will have a significant impact on the assembly state of the composite bolted joint and result in the joint strength deviating from the design value. This is a key bottleneck in improving the performance of composite bolted structures. Existing related studies have given less consideration to initial assembly deviations, usually focusing on the effect of a single deviation when it acts alone. In fact, there is a significant coupling effect of multi-source shape-position deviations on the assembly results and joint strength. In this study, a fast prediction method for the strength of the composite bolted joints considering the effects of initial shape-position deviation is proposed. This method firstly quantitatively expresses, and data fuses the multi-source initial assembly deviation information of the composite bolted joint. Using the fused deviation information as input, the joint strength is obtained through the virtual assembly-loading analysis. Prepare datasets by parametric sampling and batch simulation. Construct a neural network model and train it using this dataset. Finally, the fast model for the strength prediction considering the initial shape-position deviation of composite bolted joints is established. This model can provide assistance in performance evaluation and calibration of composite bolted joints.

Data science and machine learning applications for composite materials and biomedical engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INVESTIGATING THE EFFECTS OF THE MECHANICAL VENTILATION STRATEGIES ON PULMONARY MECHANICS PROPERTIES FOR CHILDREN WITH ACUTE RESPIRATORY DISTRESS SYNDROME

Siang-Rong Lin[*1], Jeng-Hung Wu[2], En-Ting Wu[2] and Chia-Ching Chou[1]*

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[2]National Taiwan University Hospital

ABSTRACT

This study aims to investigate the mechanical ventilator support management and pulmonary physiological characteristics of pediatric patients with Acute Respiratory Distress Syndrome (ARDS) in the Pediatric Intensive Care Unit (PICU).

The lung parenchyma of patients with ARDS often exhibits inhomogeneity, leading to local stress concentration and causing local lung injury, triggering a local inflammatory response. Pulmonary recruitment maneuvers, such as the application of positive end expiratory pressure (PEEP), are common treatments for patients with ARDS. Pulmonary recruitment involves the sustained application of pressure in the airways, allowing collapsed alveoli to reopen. This not only improves oxygenation in patients with ARDS but also helps prevent shear injuries caused by the repetitive opening and closing of alveoli. However, excessive PEEP can also cause lung damage, leading to Ventilator-Induced Lung Injury. At present, the optimal PEEP setting strategy remains unclear and has not yet been determined.

Therefore, we collect ventilator settings records and pulmonary compliance and inflammation evaluation data from patients with ARDS in the PICU. Through data processing and machine learning (including supervised learning and reinforcement learning), we evaluate the impact of different ventilator settings on lung compliance. Additionally, we apply the Ontology Web Language to encode the structural information of respiratory system anatomy and pulmonary mechanics, integrating this information into the machine learning models to enable them to learn from these data. This analysis enhances our understanding of how strategies of mechanical ventilator influence the physiological status of patients, providing more concrete guidance for clinical practices.

UPPER AND LOWER BOUNDS CONFIDENCE BAND COMPUTING FOR ACCURACY AND ERROR ESTIMATION USING SEFEA (STRAIN-ENRICHED FINITE ELEMENT ANALYSIS) FORMULATION

Theodore Lin[1] and Yu Hou*[2]

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ABSTRACT

Sefea (Strain-Enriched Finite Element Analysis) formulation[1] has been incorporated into several Industrial CAE products for design analysis for over a decade now. In the latest update, Sefea further refines the enrichment method by incorporating the nodal/element cluster density into the heterogeneous enrichment process. Additional convergence in accuracy is observed even with extremely coarse meshes.

Sefea technology allows general users with minimum or no FEA experience to perform routine design analysis with ease and achieve accurate and robust results. Experienced analysts can leverage speed, accuracy, convenience, and robustness to achieve superior outcomes. As CAD design analysis becomes more prevalent, users are increasingly seeking more guidance on the accuracy and reliability of the analysis results. This is the motivation for the ongoing research.

We first review the Sefea formulation and the critical nature of the zero integral-sum of the enriched strain. The method preserves the constant stress state required for convergence while elevating the low-order constant strain tetrahedron and triangle elements to the 2nd-order element accuracy without additional equations.

We observed that the lower and upper bounds of a given mesh can be derived from the enrichment process in the optimal strain enrichment development[2]. Without any enrichment, the method effectively degenerates into a constant strain low-order element with over-conservative results. Conversely, when uniformly enriched, it exhibits a softened behavior similar to the nodal integration method[3]. In comparison, the proposed enrichment formulation selectively enriches the strain during the integration process based on nodal density, element clustering, and strain variations and produces optimal results within the upper and lower bounds for the given discretization.

The implementation offers a quick feedback on the solution bounds and accuracy with small computational costs by adjusting only the enrichment component without the need for a costly element integral loop. It greatly improves the usability and accuracy projection for general CAE design analysis.

We will present the comparison with the analytical and other numerical methods, evaluating the accuracy, computational efficiency, and general usability. Comparison with traditional error evaluation techniques such as the energy error method is also reviewed. Finally, we highlight the potential areas for future research and development.

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Geometric mechanics formulations and structure-preserving discretizations for continuum mechanics and kinetic models
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DISTRIBUTIONAL COMPLEXES AND THEIR COHOMOLOGY: HESSIAN, DIVDIV, AND ELASTICITY

Ting Lin[*1], Kaibo Hu[2], Qian Zhang[3] and Snorre Christiansen[4]*

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ABSTRACT

Recently, there has been a growing interest in discretizing differential complexes beyond the de Rham case, including the Hessian, divdiv, and elasticity complexes. A conforming finite element discretization may involve high polynomial degrees. In contrast, using distributional spaces is much more computationally efficient. Moreover, distributional spaces can be categorized as elements from the dual mesh, which formally establishes a connection between finite element exterior calculus and discrete exterior calculus.

In this talk, I will discuss the distributional Hessian, divdiv, and elasticity complexes and their cohomologies in both 2D and 3D settings. We will prove that the cohomologies are isomorphic to their continuum counterparts. For the Hessian and divdiv complexes, we will first construct the discretization. As for the elasticity complex, we will delve into the Regge complex. Additionally, we will explore the twisted complex of the Regge complex, which can be seen as a differential complex perspective of the microstructure elasticity model.

A HIGHLY PARALLEL SIMULATION OF PATIENT-SPECIFIC HEPATIC FLOWS

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ABSTRACT

Computational hemodynamics is being developed as an alternative approach for assisting clinical diagnosis and treatment planning for liver diseases. The technology is non-invasive, but the computational time could be high when the full geometry of the blood vessels is taken into account. Existing approaches use either one-dimensional model of the artery or simplified three-dimensional tubular geometry in order to reduce the computational time, but the accuracy is sometime compromised, for example, when simulating blood flows in arteries with plaque. In this work, we study a highly parallel method for the transient incompressible Navier-Stokes equations for the simulation of the blood flows in the full three-dimensional patient-specific hepatic artery, portal vein and hepatic vein. As applications, we also simulate the flow in a patient with hepatectomy and calculate the portal pressure gradient. One of the advantages of simulating blood flows in all hepatic vessels is that it provides a direct estimate of the portal pressure gradient, which is a gold standard value to assess the portal hypertension. Moreover, the robustness and scalability of the algorithm are also investigated. A 83% parallel efficiency is achieved for solving a problem with 7 million elements on a supercomputer with more than 1000 processor cores.

Constitutive modeling of complex materials with machine learning and artificial intelligence
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A TWO-STEP CONSTITUTIVE MODELING FRAMEWORK BASED ON DATA-DRIVEN IDENTIFICATON AND PHYSICS-AUGMENTED NEURAL NETWORKS

Lennart Linden[*1], Karl Kalina[1], Jörg Brummund[1] and Markus Kästner[1]*

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ABSTRACT

The formulation and calibration of constitutive models remain a difficult task for materials that exhibit complex nonlinear elastic or inelastic behavior. Therefore, new approaches, generally referred to as data-based or data-driven methods, have become increasingly popular in the computational mechanics community in recent years. However, these approaches require a large amount of data, usually stresses and strains for problems in solid mechanics. In this contribution, we present a consistent two-step approach for the automated calibration of hyperelastic constitutive models which only requires experimentally measurable data.

In the first step of our approach, data-driven identification (DDI) is applied to determine tuples consisting of stress and strain states [1]. This method enables to identify these data by only prescribing the applied boundary conditions and the displacement field which can be determined from full-field measurement methods such as digital image correlation (DIC). In the second step of the proposed framework, the data are used to calibrate a physics-augmented neural network (PANN) [2]. This model fulfills all common conditions of hyperelasticity by construction and is very flexible at the same time. The implementation of the PANN model into a finite element (FE) code is straightforward.

We demonstrate the applicability of our approach by several descriptive examples. Therefore, two-dimensional synthetic data are exemplarily generated by using a reference constitutive model. The calibrated PANN is then applied in three-dimensional FE simulations, where the solution is compared to the reference model.

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BAYESIAN MULTIMODEL INFERENCE IN SYSTEMS BIOLOGY AND MEDICINE

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ABSTRACT

When modeling biological systems, one must often choose from several possible models based on different sets of simplifying assumptions and theories. However, conditioning predictions on a specific model formulation can introduce uncertainty and bias due to the selection of one particular model. Thus, to ensure accurate prediction and uncertainty quantification, we must account for uncertainty in the model formulation in the resulting predictions.

Model selection and discrepancy modeling approaches allow one to choose the “best” model and directly account for model uncertainty. However, given the limited data in many biological applications, these approaches may lead to biases due to the selection of a single model. In this talk, we highlight several methods for multimodel inference that leverage the entire set of available models to avoid selection biases and account for model uncertainty by incorporating contributions from all models. Methods including Bayesian model averaging, pseudo-Bayesian model averaging, and stacking of predictive densities construct robust predictors using the entire model family and avoid conditioning predictions on one model.

In this talk, we characterize multimodel inference with several examples from systems biology, including mitogen-activated protein kinase (MAPK) signaling and prediction of pancreatic function for diabetes diagnosis. Our results show how multimodel inference accounts for model uncertainty and, thus, improves predictive certainty and reduces model selection bias. Furthermore, we demonstrate how multimodel inference yields models that better agree with experimental data and provide more reliable predictions.

Current trends in phase-field modeling and computations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MULTISCALE ANISOTROPIC POLYMER NETWORK MODEL WITH PHASE FIELD FRACTURE AT FINITE STRAINS

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ABSTRACT

This presentation focuses on modeling fracture in rubber-like materials. Our study proposes a multiscale fracture model for elastomers, considering isotropic and anisotropic network responses, using the non-affine microsphere model and the maximal advance path constraint network model, respectively [1,2]. For the latter, macroscale fracture is driven by micromorphic regularization, introducing local-global damage variables. The model is validated using double-edge notched tensile tests and compared with experimental data. Uniaxial tensile experiments on PDMS rubber films with notches are conducted, and simulations are compared with experimental observations. Visualization of stretch and damage evolution in chains oriented differently assesses predictive capacity. Results are compared with alternative models, demonstrating the utility of our approach in accurately simulating rubber-like material fracture behavior.

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Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SOME STRUCTURES PRESERVING KERNEL-BASED METHODS

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ABSTRACT

In this talk, we present innovative kernel-based meshless methods devised to preserve critical structures when solving Hamiltonian and dissipative PDEs. Our first method introduces a conservative Galerkin approach with radial basis functions for Hamiltonian wave equations, ensuring energy conservation through projection operators and a second-order average vector field scheme. The second method details a meshless Galerkin technique for dissipative PDEs on surfaces, which upholds energy dissipation inherently. Both methods are supported by rigorous error and convergence analyses, and their effectiveness is demonstrated with numerical experiments, confirming their theoretical properties.

Constitutive modeling of complex materials with machine learning and artificial intelligence
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ON THE ROLE OF INTERPRETABILITY OF DATA-DRIVEN CONSTITUTIVE MODELING BY CONSTITUTIVE ARTIFICIAL NEURAL NETWORKS

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ABSTRACT

The classical, theory-driven approach to describe the deformation of a material body relies on the formulation of constitutive equations relating strains and stresses. A drawback of this approach are the efforts typically required to develop appropriate functional relations and identify material parameters .

These efforts are not required in data-driven approaches to constitutive modeling. To combine the advantages and overcome the disadvantages of both theory- and data-driven constitutive modeling, we have developed the novel concept of Constitutive Artificial Neural Networks (CANNs). This machine learning approach to data-driven constitutive modeling does not require any major a priori assumptions about the constitutive law but yet incorporates substantial theoretical knowledge about continuum mechanics and constitutive theory. This way, CANNs are able to learn the constitutive law of a material from relatively small amounts of stress-strain data. Moreover, our results suggest that CANNs can robustly discover various flavors of material models from data and by design have clear physical interpretation. These abilities will be illustrated using various data collected from arterial and brain tissue.

New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION APPLIED TO PROBLEMS WITH LOCAL FATIGUE CONSTRAINTS BASED ON AUGMENTED LAGRANGIAN METHOD

Carlos Eduardo Lino[*1], Emilio Carlos Nelli Silva*[1] *and André Luis Ferreira da Silva*[1]

[1]*University of São Paulo*

ABSTRACT

Authors:Carlos Eduardo Lino, André Luis Ferreira da Silva, Emilio Carlos Nelli Silva

Fatigue is the most usual failure mode of any mechanical structure subject to loading. There are several methods to predict the structure life, and different approaches can be applied to extend this life. From the point of view of materials engineering, new materials can be proposed to deal with this issue. However, developing and producing these materials can be expensive. A different approach consists of optimizing the design using some optimization algorithm, determining the optimized material distribution that ensures a higher fatigue life. This work proposes to use topology optimization to design structures subjected to permanent loads to increase the component life. The objective is to minimize the volume, considering fatigue constraints. The works in the literature deal with fatigue constraints using aggregate methods, which are common in problems considering stress constraints. Our proposed approach uses a norm of the stress field to represent the stress constraint. However, stress and fatigue are local phenomena. Thus, in this work, the Augmented Lagrangian method is used to deal with the large number of constraints in the problem. This approach, previously used in stress-constraints problems, makes treating fatigue as a local phenomenon. The Modified Goodman method is used to measure local fatigue. This method considers a sensitivity factor that accurately estimates fatigue life. Numerical examples show the efficiency of the proposed method.

Computational mechanics for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RESIDUAL STRESSES COMPUTATION AND OPTIMIZATION FOR DIRECTED ENERGY DEPOSITION PROCESSES

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ABSTRACT

The adoption of metal additive manufacturing by various industries is being hindered by the presence of residual stresses and distortion in the deposited parts. One of the important challenges that hinder the adoption of metal AM parts is the formation of residual stresses. Layer-by-layer deposition during metal AM causes cyclical heating and cooling of the metal deposit, resulting in the formation of residual stresses [1]. The presence of residual stresses is often undesirable as it could lead to delamination and cracking of deposited parts. Parameter optimization is predominantly used for residual stress mitigation. Finite Element Analysis (FEA) is a valuable tool for predicting residual stresses, but it requires substantial computational power. Direct energy deposition (DED) is a promising additive manufacturing technique that enables the fabrication of complex structures with excellent mechanical properties. This study aims to reduce computational time by incorporating a thermo-mechanical model specifically designed for the DED processes. This model predicts the thermal history and subsequent residual stresses in the deposited material. Various FEA methods are examined to provide a comparative analysis of computational cost and numerical accuracy. These findings contribute towards the realization of a faster modeling approach, where the incorporation of efficient and accurate FEA models can optimize part quality and strength while reducing computational time.

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Numerical modelling of composite materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ELASTIC-PLASTIC SEMI-ANALYTICAL METHOD AND OPTIMIZATION FOR CURVED SCARF BONDING REPAIRS OF COMPOSITE STRUCTURES

Bin Liu[1] and Yancheng Liu*[1]

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ABSTRACT

For the semi-analytical method, Hart-Smith[1] first derived a two-dimensional analysis model for scarf repaired and step repaired isotropic materials. Basing on this method, Harman and Wang[2] introduced average reduction method of composite section elastic modulus, and derived a method for calculating stress distribution of two-dimensional scarf repaired composites. Additionally, they proposed an optimization method to minimize the peak shear stress of adhesive layer by optimizing the bonding angle distribution controlled by first order equation. To restore the stress concentration caused by the change of angles of fiber orientation accurately, Liu[3] improved the method with stiffness-distribution principle and provided a modified analytical method(MAM), which has achieved a more precise and believable result in calculating stress distribution on flat adhesive surfaces. MAM and the application of stiffness-distribution principle has been proven concise effective by Yan[4] with experiments.

In this paper, a semi-analytical stress distribution calculating method that is applicable to arbitrary shape surfaces of scarf repaired composites are proposed. To take not only the cohesive failure caused by shear stress, but also the yield of adhesive under consideration, the adhesive is regarded as an elastic-plastic material. Furthermore, an optimization algorithm basing on this method which could significantly improve the carrying capability of scarf repaired composite laminates is developed. Several examples have revealed high universality and accuracy of this method, and the optimization algorithm developed from which has achieved an excellent effect on reducing peak shear stress. Although it would be difficult to manufacture the optimized surface, this paper still provides a simple but efficient way to evaluate designs of scarf repair and reliable schemes for advancing carrying capacity of scarf repaired composites.

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Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A HIERARCHICAL QUADRATURE ELEMENT METHOD FOR FRACTURE PARAMETERS CALCULATION AND CRACK PROPAGATION SIMULATION

Bo Liu[*1], Pai Xu[1], Siqi Jia[1] and Wei Xiang[2]*

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ABSTRACT

This paper presents a hierarchical quadrature element method (HQEM) with p-convergence for the calculation of fracture mechanical parameters and the simulation of crack propagation with very coarse meshes and high accuracy and efficiency. The stress intensity factor (SIF), strain energy release rate (SERR), J-integral and weight function are computed using minimum mesh refinement and high accuracy. The SERR is directly computed though virtual crack closure method (VCCM) with high accuracy. Although extrapolation is needed in computing SIF and J-integral, they can also be automatically obtained by choosing a certain local mesh size. The computed fracture mechanical parameters are then used to simulate crack propagation using minimum number of elements. The number of elements is significantly reduced through interpolating the crack trajectory as a single curve and modelling the opened crack as two elements only. Thus, the number of elements is unchanged in the whole simulation process, which greatly improves the computational efficiency. The feasibility of applying the HQEM to fracture mechanical parameters computation and crack propagation simulation is demonstrated through several benchmark examples of mode I and mode II fractures (or mixed mode) with homogeneous materials as well as bimaterials. Numerical comparisons with available results in literatures validated the high accuracy and efficiency of the HQEM, which indicates it has promising potential for complex large-scale fracture problems.

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Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SIGNED DISTANCE FIELD ENHANCED VIRTUAL ELEMENT METHOD FOR LARGE DEFORMATION FRICTIONAL CONTACTS IN FLEXIBLE MULTI-BODY SYSTEMS

Chuanqi Liu[*1]

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ABSTRACT

We propose the signed distance field virtual element method (SDF-VEM), which is a virtual element method variant able to model large deformation frictional contact problems in flexible multi-body systems with signed distance field assisted as a geometrical tool. Leveraging the geometrical versatility inherent in the virtual element method, we could represent each flexible body with either a single-element or a multi-element polygonal mesh of arbitrary shape. This enables node-to-node contact enforcement through adaptive mesh insertion and adjustment. Addressing the complexity of contact detection scenarios in multi-body models, arising from the irregular shapes and numerous bodies involved, we introduce an SDF-assisted unified and automatic contact detection framework. Numerical examples in 2D, including Hertzian contact, spur gears engagements, and granular particles contacts, demonstrate the accuracy and effectiveness of our method.

Multiphysics biomechanics of bio- and bio-inspired soft materials: Theory, simulation and experiments
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GRADIENT-ENHANCED MODELING OF PORO-VISCO-HYPERELASTICITY-INDUCED TIME-DEPENDENT FRACTURE OF BLOOD CLOTS

Dongxu Liu[*1], Nhung Nguyen[1] and Luka Pocivavsek[1]*

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ABSTRACT

A blood clot is a natural soft tissue composed of fibrin networks, red blood cells, and platelets. It contributes to hemostasis when it forms on wounded blood vessel walls, while intravascular clots can cause pathological thrombosis. Due to complex physiological loading, their fracture resistance is crucial for physiological hemostasis and pathological thrombosis. However, the mechanism of blood clot fracture is still not well understood. Quantifying blood clots' deformation and fracture is essential for diagnosing and treating bleeding disorders and thrombotic diseases. This work aims to formulate a thermodynamically consistent, multi-physics theoretical framework for describing blood clots' time-dependent deformation and fracture. This theory concurrently incorporates fluid transport through porous fibrin networks, non-linear visco-hyperelastic deformation of the solid skeleton, solid/fluid interactions, mechanical degradation of tissues, gradient enhancement of energy, and protein unfolding of fibrin molecules. The constitutive relations of tissue constituents and the governing equation of fluid transport are derived within the framework of porous media theory by extending non-linear continuum thermodynamics at large strains. A physics-based, compressible network model is developed to describe the mechanical response of the fibrin network of blood clots. The kinetic equations of the internal variables, introduced for describing the non-linear viscoelastic deformation, non-local damage driving force, and protein unfolding, are formulated according to the thermodynamics principles by incorporating a non-equilibrium energy of fibrin networks, a gradient-enhanced energy, and a stretch-induced internal energy of fibrin molecules, respectively, into the total free energy density function. An energy-based damage model is developed to predict the damage and fracture of blood clots. The proposed model is implemented into finite element code by writing subroutines and is experimentally validated using single-edge cracked clot specimens with different constituents. Computational results show that this model can accurately capture the experimentally measured deformation and fracture. The fracture of blood clots subjected to multiple loading conditions is simulated, and the results demonstrate that the deformation and fracture are sensitive to loading rate. The tissue subject to a higher loading rate is stiffer. The damage at the crack tip initiates earlier and propagates faster when the loading time approaches the characteristic time of intrinsic viscoelastic. The fluid transport influences the fracture by tissue swelling. The mechanisms of blood clots fracture are analyzed systematically. The results hypothesize the importance of fibrin network viscoelasticity and fluid transport in the stability of blood clots.

Physics-based data-driven modeling and uncertainty quantification in computational materials science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CORRELATION-BASED LIKELIHOOD-FREE CALIBRATION FOR REALISTIC INVERSION OF MODEL UNCERTAINTY PARAMETERS

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ABSTRACT

The Computational model is widely used to represent physical process property, but the prevalence of uncertainty leads to a failure to match the two. Calibration is often used to tune unknown calibration parameters of a computational model. However, model discrepancy can exist even if all calibration parameters are known. One of the main challenges in model calibration is the difficulty in distinguishing between the effects of calibration parameters versus model discrepancy. Thus, the paper illustrates in detail the reason for the identifiability problem of existing methods, and based on this, we propose a new concept that the computational model and the real physical process should be “the most similar” rather than “the closest”. Further, we propose the correlation-based likelihood-free calibration, which avoids the difficulty of solving the maximum likelihood function while obtaining the most realistic calibration parameters. By comparing all the basic function cases and one common engineering case with the existing methods, the results show that our proposed method can obtain a realistic inversion of the model parameters, and the consistency of the parameters will also significantly improve the prediction accuracy of the model.

Multi-scale, multi-rate damage and fracture: Models, experiments, and simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NOVEL DUCTILE FRACTURE PREDICTION OF ADDITIVE MANUFACTURED TI6AL4V ALLOY

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ABSTRACT

Selective Laser Melting (SLM) is one of the revolutionary additive manufacturing (AM) technologies to produce metallic mechanical parts. To thoroughly understand the damage and fracture behavior of SLM-fabricated Ti6Al4V alloy under complex stress states, the article conducted experimental and simulation studies on various types of Ti6Al4V alloy specimens. By incorporating a novel stress state function into an enhanced GTN (Gurson-Tvergaard-Needleman) model, the study successfully predicted the ductile fracture behavior of the Ti6Al4V alloy.

(1) A number of tensile, compressive and torsional experiments covering various stress states were conducted with different types of the specimens, the study has clearly identified the failure modes under different stress states.

(2) A modified GTN model developed by the Authors' team was adopted in the ductile fracture analysis of SLM-fabricated Ti6Al4V alloy. The introduction of a shear damage variable and a stress state-dependent function extends the application of GTN model to a broader range of stress states.

(3) A parameter calibration strategy of the dual damage variable GTN model was proposed, based on the finite element inverse analysis and referring to a group of experimental results. These parameters encompass quenching parameters and damage parameters, with the latter consisting of 6 parameters related to void volume fraction, 4 parameters related to shear damage, as well as 1 parameter within the stress state function. The applicability of the parameters was well validated via the simulation of another group of experiments.

(4) The morphologies of the fracture surfaces were successfully predicted by using the developed damage constitutive model, and the results demonstrated that the deformation, strength and fracture modes of SLM-fabricated Ti6Al4V alloy can be well described by the developed dual damage variable GTN model. Both damage variables contribute to the different failure mechanisms. The variable of void fraction controls fibrous zone failure based on the void growth mechanism, and the shear damage variable facilitates shear fracture based on the void shear mechanism.

Imaging and computational methods for biomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INCREASED POWER OF HEMODYNAMIC LOW-FREQUENCY OSCILLATIONS CAN IMPROVE CEREBRAL OXYGENATION

Shilin Yang[1], Pandeng Zhang[1], Zhixian Zhang[1], Xinyu Chen[2], Xia Long[2], Yanxia Zhou[2] and Jia Liu[1]*

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ABSTRACT

Cerebral hemorrhage or ischemia can significantly increase the low-frequency oscillations of blood pressure and cerebral blood flow. Recent studies have shown that such low-frequency oscillations can improve the brain's oxygenation even in the context of reduced cerebral blood flow, which necessitates further investigation. However, this type of study requires special devices, and although previous results have suggested an increase in cerebral oxygenation associated with low-frequency oscillations, it is still unclear whether this increased oxygenation requires a certain power of low-frequency oscillations. We therefore designed and carried out this study.

We recruited 11 healthy subjects aged 18-30 years old, and the experiment was carried out at the Second People's Hospital of Shenzhen. Using the routine clinical syncope test procedure, each participant completed four consecutive stages of the test on a tilt table for syncope testing, including: 10 minutes of supine rest, then the tilt table was raised to a 70-degree angle from the ground within 6 seconds, maintained for 20 minutes, followed by oral administration of 0.25 mg of nitroglycerin, continuing for another 20 minutes, and finally returning to the initial supine position. During the test, we continuously collected blood pressure, bilateral middle cerebral artery blood flow velocity using transcranial Doppler, and near-infrared cerebral blood oxygen signals. Subsequently, we analyzed changes in the power of low-frequency oscillations using power spectral analysis of continuous blood pressure and cerebral blood flow velocity, and calculated changes in the cerebral oxygenation index based on the cerebral oxygen signal.

Our study found that the participants' cerebral blood flow velocity gradually decreased from supine (62.74±1.11 cm/s) to upright (55.65±1.83 cm/s, $P<0.05$) position, and then further after nitroglycerin administration (upright: 55.65±1.83 cm/s vs drug: 43.46±3.93 cm/s, $P<0.05$). At the same time, the power of hemodynamic low-frequency oscillations at approximately 0.1 Hz frequency progressively increased (supine: 45.37±31.38 (cm/s)2Hz-1 vs upright: 133.33±55.71 (cm/s)2Hz-1, $P<0.05$; upright: 133.33±55.71 (cm/s)2Hz-1 vs drug: 243.19±98.82 (cm/s)2Hz-1, $P<0.05$). Interestingly, although the change in cerebral oxygenation index during the upright phase was consistent with the trend of decreasing cerebral blood flow, the cerebral oxygenation index significantly increased when low-frequency oscillations were further enhanced after taking nitroglycerin (upright: 0.0101±0.0008 μM vs drug: 0.0128±0.0008 μM, $P<0.05$).

Therefore, our study suggests that the routine clinical syncope test can effectively induce hemodynamic low-frequency oscillations. We observed for the first time that the increase in cerebral oxygenation index is related to the power of low-frequency oscillations.

Physical models and reduced order models augmentation with data for physics-informed machine learning in real-world applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ENHANCING PREDICTIVE MODELING IN REACTOR BUILDING DOSE DISTRIBUTION: A NEURAL NETWORK-AIDED APPROACH

Jihong Liu[1], Koji Koyamada[1], Hiroaki Natsukawa[1] and Shuhei Kamioka[1]*

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ABSTRACT

Theoretical predictions of dose distribution inside a reactor building using Boltzmann transport equation present a computational challenge due to its substantial resource requirements [1]. To address this issue, we simplify the approach to a diffusion equation in situations where the mean free path of neutrons is relatively short, assuming random scattering [2]. This simplification enhances the manageability of calculations, particularly in scenarios where the scale of computational demands makes Boltzmann equation impractical.

This study involved altering the building shape and radiation source to calculate the Boltzmann transport equation. This methodology enables us to consider various scenarios and conditions influencing neutron transport within the reactor building. The obtained results were then used to derive the diffusion equation through a neural network based on physical information [3]. The incorporation of a neural network introduces computational efficiency and adaptability, thereby improving the practicality of the diffusion equation approach.

The distribution of derivation errors within the building space was visualized, aiding in comprehending the model's accuracy. This visualization highlights areas where the derived diffusion equation may deviate from the more computationally intensive Boltzmann transport equation. The identified regions where the diffusion equation approximation is effective offer valuable insights for practical applications, guiding users on when and where this simplified approach can yield accurate results.

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Advanced materials and smart structures: Modeling, simulation and testing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A CONTINUUM AND COMPUTATIONAL FRAMEWORK FOR NONLINEAR VISCOELASTICITY: BEYOND THE HOLZAPFEL-SIMO APPROACH

Ju Liu[1], Jiashen Guan[1], Chongran Zhao[1] and Jiawei Luo[1]*

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ABSTRACT

Viscoelasticity is a ubiquitous mechanical property in soft matter. The constitutive and computational modeling of nonlinear viscoelasticity is particularly relevant to the understanding and prediction of the performance of various engineering and biomedical materials. There are several desirable features in the design of a model: the soundness in its theoretical root; the potential in accounting for additional materials features (e.g., anisotropy, damage, etc.); the capability to faithfully represent material behavior using as less parameters as possible; the convenience of finite element implementation.

The Holzapfel-Simo model [1] has gained popularity over the past several decades, mainly because it is amenable to finite element implementation and convenient in accounting for material anisotropy. The lack of a thermodynamic foundation has been viewed as a major drawback of this model. In our recent work, we constructed a complete thermomechanical theory for this model and thereby addressed previous concerns [2]. In particular, the study elucidates the origin of the evolution equations of the non-equilibrium stress. It also emphasizes the importance of satisfying the relaxation property for the free energy in the equilibrium limit.

Interestingly, our analysis also reveals that the Holzapfel-Simo model can be regarded as a theory built based on the Green-Naghdi kinematic assumption and the St. Venant-Kirchhoff model for the non-equilibrium elastic behavior. Based on this observation, we extend the Holzapfel-Simo model by incorporating nonlinear effects. A two-parameter strain measure family, which incorporates the well-known Seth-Hill strain family, is introduced. The Green-Naghdi kinematic assumption allows a convenient modular modeling strategy for the inelastic effects using the generalized nonlinear strain measures.

A suite of combined numerical methods is proposed for the computational modeling of the viscoelasticity model. In particular, a smooth generalization of the Taylor-Hood element based on Non-Uniform Rational B-Splines serves as the element technology and is used within a generalized Herrmann mixed variational formulation. A class of strain-drive constitutive integration schemes is discussed, which allows the energy-consistent integration of the overall system. Analysis results and numerical examples will be provided to justify the effectiveness of the proposed methodology.

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Uncertainty quantification and reliability analysis in engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RELIABILITY DESIGN OF MONOPILE FOUNDATIONS IN SPATIALLY VARIABLE SOIL CONSIDERING RANDOM LOADS

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ABSTRACT

Due to the spatial variability of soil properties and the uncertainty of marine environmental loads caused by wind, waves and currents, it is indispensable to perform reliability-based design of monopiles that are extensively utilized in the offshore wind industry. In this study, the random individual capacities and probabilistic VHM failure envelopes of monopiles in spatially variable undrained soil are first obtained using the random finite element method combined with Kriging meta-modelling technique and Monte Carlo simulation. Then, the relationship between the appropriate design (characteristic) quantile of soil shear strength and normalized scale of fluctuation and coefficient of variation of soil strength is investigated when considering the spatial variability of soil as well as the uncertainty of loads. Finally, a design framework of monopiles using appropriate design quantile of soil strength is proposed and verified via an example. The results show that the designed monopile can not only meet the two reliability design requirements set in DNV (2013), but also significantly save costs. The study could be helpful to the design of monopile foundations in practical engineering.

MATHEMATICAL MODELING AND NUMERICAL SIMULATION OF MECHANICAL-THERMAL-CHEMICAL MULTI-FIELD PROCESS

Ke Liu[1], Yazhi Li[1] and Biao Li[1]*

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ABSTRACT

Solid materials are subjected to the interactions of multiple physical and chemical fields when they serve in extreme environments. Their response, such as deformation, mass transfer, heat transfer, and chemical reactions, is intimately related to the failure of structures. Multi-field coupling problems implicate interactions among different physical and chemical fields. Considering the multi-field coupling problem which were affected by the force, heat and chemistry, involves complex dynamic process of multi-component substance in an open system, this work chosen a macroscopically homogeneous body composed of a chemically active medium as the research object. And the force balance, mass balance, and internal energy balance equations were provided based on the fundamental laws of thermodynamics. A fully coupled constitutive model that combines mechanical, thermal, diffusion, and chemical reaction effects was then developed to describe the intricate interplay between these effects. The inertial effects of force, entropy and chemical potential were introduced into a macroscopic uniform body by considering the propagations of elastic waves, temperature waves and diffusion waves. Considering the various influential mechanisms, the contributions of mass diffusion and chemical reaction were separated. The evolution equations of heat conduction, diffusion, and chemical reaction were constructed according to the energy dissipation inequality. This coupling model can effectively describe the transient evolution and quasi-static response of multi-field coupled system. Furthermore, the weak form of governing equations were derived by applying the chemical Gibbs function variational principle, which is based on the universal variational principle of thermodynamics. In particular, the model has the ability in predicting the concentration and entropy jump conditions on the moving interface.
In order to verify the proposed model, the oxidation process of silicon nitride was numerically calculated, and the evolutions of oxide thickness and stress were presented. The results agree with the reference results, indicating that the mechanical-thermal-chemical multi-field coupled model is able to reflect the evolution laws of the stress field, concentration field, temperature field and displacement field of silicon nitride under the coupling effect of multi-physical fields.

Model-based simulations of structural responses under extreme conditions
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NOVEL GPU IMPLEMENTATION OF NONLINEAR EXPLICIT DYNAMIC ANALYSIS FOR COMPLEX CIVIL STRUCTURES

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ABSTRACT

The explicit integration method is recognized as the main approach for solving nonlinear transient dynamic responses involving material failure and large deformation. Since computation of the explicit integration is intrinsically decoupled, an efficient implement should consider parallel acceleration, especially GPU acceleration. However, there are still some challenges using GPU as the accelerators when large structures contain multiple element types or complex material constitutive models. To this end, this work presents a novel GPU acceleration strategy for explicit integration method for complex structures.

A basic parallelized computational framework is established using the Compute Unified Device Architecture (CUDA). All stages of the explicit dynamic analysis are ported to GPU, including calculating element strains, stresses and internal forces, assembling the nodal effective force and solving the kinetic equations for nodes at every time step. CPU is responsible for data output. Data transfer between the CPU and GPU is necessary only at the output time step. A concurrent execution strategy is designed to solve problems with non-uniformity of element and material types. The FE model is decomposed into a few domains depending on element or material types as well available memory. The aforementioned parallel computing processes for each domain are performed concurrently on GPU. Once the computation of nodal effective forces at each time step of all domains finishes, data communication between different domains is achieved using MPI. Different data for computation mainly reside in global memory, which is the largest memory available on GPU. These data have to be organized in optimal layouts to allow the coalesced memory access. In our data structure, data for elements and nodes are organized in structure-of-arrays. Element matrices with identified size and sparsity in one domain are rearranged as a collection of arrays with each array corresponding to the values at the same matrix position. Additionally, loop unrolling strategy are employed to reduce instruction latency on GPU. Data in one domain are divided into sets with each set of the same size as the thread block. A block with n threads treats p data sets with n entries, each thread handles entries in the same position in p data sets within one execute iteration.
Performance tests from engineering designs show that a speedup of more than 40 is achieved compared to the CPU serial code computing by commercial YJK building software with validated accuracy of the results.

Emerging frontiers and methods in digital manufacturing: Modeling, simulation, and beyond
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MICROSTRUCTURAL CONTROL AND DEFECT ANALYSIS FOR FLOW-MEDIATED CRYSTALLIZATION USING PHYSICS-INFORMED DEEP LEARNING

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ABSTRACT

Crystallization, more generally, liquid-solid phase transitions, is a ubiquitous process of significance for industries ranging from manufacturing to pharmaceuticals. Defect analysis and quality control of crystal microstructure are most important in those processes. To that end, reliable and efficient techniques that can give insight into controlling parameters for achieving desired crystal microstructures are critical. Recently, physics-informed neural networks (PINNs) have shifted the paradigm for scientific computing as a data-efficient computational tool for solving scientific inverse problems.

Based on a novel phase field crystal (PFC) formalism, we will discuss how we construct PINNs to identify key parameters controlling crystallization for systems such as CsPbI_3 perovskites. We will also demonstrate the validation and capability of the inverse problem solver for identifying crystal-level controlling strategies for defect mitigation based on first-principle synthetic data and real experimental data.

Deep and machine learning methodology in the context of application to computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT AND EVALUATION OF MG-CA DEEP LEARNING INTERATOMIC POTENTIALS WITH AID OF AB-INITIO CALCULATIONS

Lijun Liu[1] and Yoji Shibutani*[1]

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ABSTRACT

Key Words: Interatomic Potential, Mg-Ca alloys, First-principles calculations, Molecular dynamics, Deep learning.

Ab initio molecular dynamics (AIMD) has become a significant tool for microscopic understanding of a wide range of problems. However, the spatial and temporal scales that AIMD can access are limited. Most AIMD calculations can only handle systems containing hundreds of atoms on picosecond timescales. On the other hand, conventional molecular dynamics (MD) can be computed efficiently, but its accuracy is limited to empirically determined atomic interaction potentials.

Nanocrystalline structures of metals, which are real-world applications, are composed of tens to hundreds of millions of atoms, which is far beyond the capabilities of ab-initio calculations. However, the main problem with empirical potentials is the need for more accuracy for structures with defects, such as point defects, dislocations, nanoclusters, etc. Therefore, the development of interatomic potentials with high accuracy is crucial.

Recently, some experimental [1] and molecular dynamic results [2] have reported that the ductility of Mg alloys is improved by the solid solution of Ca. In the design of high-performance Mg-Ca alloys, besides the solid solution effect of Ca atoms, the interactions of dislocations, twins, and grain boundaries with microstructures such as Ca solid solution clusters and precipitates are also essential factors to be considered [3]. Most developed Mg-Ca potentials can reproduce some basic properties under an equilibrium state. However, these potentials are not able to give accurate predictions when the state is unstable or defects are included. The present study used datasets from ab-initio calculations to develop Mg-Ca interatomic potentials by deep learning. Our developed Mg-Ca deep potentials can accurately predict not only basic physical, mechanical, and thermal properties but also phase transition under high temperatures and pressures, which is not able to be done by empirical potential.

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Multi-scale, multi-rate damage and fracture: Models, experiments, and simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CREEP LIFE PREDICTION OF COATED TURBINE BLADES CONSIDERING THE INFLUENCE OF FILM COOLING HOLE BLOCKAGE

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ABSTRACT

Blockage of film cooling holes significantly impacts the operational life of coated turbine blades in harsh environments. Understanding the thermo-mechanical behavior of blades under actual film cooling hole blockage conditions is crucial for predicting failure and enhancing reliability. In this study, firstly, blockage morphologies and ratios of all film cooling holes on a full-scale turbine blade were statistically analyzed, leading to the development of a blade model incorporating blockage characteristics. Subsequently, the thermo-mechanical loads of cross-scale membrane-based structures on blades were explored using the shell conduction model and the Chaboche constitutive model. Finally, the Larson-Miller Parameter (LMP) method was adopted as the creep life evaluation criteria, considering both blocked and unblocked scenarios. The results revealed that the blockage degree of film cooling holes was lowest near the leading edge of the blade and gradually increased towards the trailing edge. Additionally, the highest temperature on the blade was located near the blade tip, with the most dangerous zone situated at the root position on the pressure surface. Blockage reduced the surface cooling efficiency and diminished the creep life, increasing the risk of blade failure. In this paper, a calculation method of cross-scale structural life model is proposed to reveal the effect of hole blockage on the creep life of turbine blades, providing valuable insights for durability assessment of coated high-temperature components.

Keywords: Turbine blade; Hole blockage; Thermo-mechanical behavior; LMP method; Creep life

Data science and machine learning applications for composite materials and biomedical engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN EXPLORATION FOR VISCOELASTIC AND DYNAMIC PROPERTY OF 2D CELLULAR MATERIALS

Li-Wei Liu[1] and Zhen-En Jian*[1]

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ABSTRACT

Cellular materials, mimicking natural architectures inside the wood and honeybee’s honeycomb, exhibit a unique combination of high stiffness and low weight. Bridging the gap in prior research on the rate-dependent and the dynamical performance of 2D cellular materials, this study proposes models and explores the viscoelastic behavior and wave propagation of 2D cellular materials. For the viscoelastic property of the material, our study finds that an increase in energy dissipation with rising relative density under strain control but a decrease under stress input. On the other hand, when the angle of cell wall increases, the strong axis of energy dissipation shifts under strain-controlled conditions. Furthermore, the anisotropic feature of energy absorption for auxetic cellular materials is observed. These results highlight the significant effects of microstructure on the viscoelastic performance of 2D cellular materials. In addition, the exploration of dynamical property of the material reveals a remarkable increase in effective Young's modulus and a significant increase in effective natural frequency when the width of cell wall approaches the characteristic material length. This enhancement is pronounced and points out the critical role of size effect in predicting dynamic responses. Moreover, our study indicates that the existence of band gaps in plane wave propagation within 2D cellular materials signifies its inherent ability to suppress energy at specific frequencies. In essence, our exploration offers insights into the intricate relationship between viscoelasticity and dynamic performance in cellular materials, emphasizing the significant influence of microstructure and size effect.

DIGITAL DESIGN OF GRINDING WHEEL FRAME OF GRINDING MACHINE

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ABSTRACT

This research paper explores the grinding wheel holder and feed mechanism to automate the grinding wheel holder. The specific objectives of this research are: (1) Through the determination of the overall programme of the grinding wheel holder of the grinding machine, the disadvantage of low processing efficiency of the ordinary grinding machine is overcome. Through the calculation and verification of the structure, including the lifting beam, serving grinding wheel spindle of the grinder, etc., the design and strength of the parts are verified to be safe and reliable through calculation and verification, and meet the design requirements. Completed the design and selection of the parts, thus improving the machining efficiency and quality of the workpiece. The grinding wheel holder structure is designed to improve the grinding efficiency of the grinding wheel, so that the grinding wheel can work smoothly in the grinder. This structural design extends the service life of the grinder and reduces costs. (2) Finite element analysis and simulation of the parts were carried out to make the structural design of the grinding wheel holder more reasonable, and to improve the reasonableness of the material and structure selection of the grinding wheel holder.

The phase field method for fracture: Theory, numerics, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ASYMPTOTIC HOMOGENIZATION FRAMEWORK FOR PHASE FIELD FRACTURE OF HETEROGENEOUS MATERIALS AND APPLICATION TO TOUGHENING

Sen Liu[*1] and Yongxing Shen*[1]

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ABSTRACT

We propose an asymptotic homogenization framework to account for the fracture of heterogeneous materials. This framework upscales the phase field model for microscale fracture and outputs anisotropic effective properties such as the degraded elasticity tensor and the fracture toughness. Furthermore, it quantitatively accounts for the toughening effect in a succinct way. More specifically, when the critical energy release rate of a heterogeneous material is uniform, the framework reveals that toughening is essentially determined by the disparity of the toughnesses, the energy absorbed by the material before cracking.

New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN INTERFACE-ENRICHED TOPOLOGY OPTIMIZATION FOR MITIGATING THE EFFECT OF SURFACE FLAWS IN 3-D BRITTLE SOLIDS

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ABSTRACT

We propose a fracture-based topology optimization procedure for tailoring the fracture resistance of 3-D brittle solids. Developing on our previous work [1], topology is described by means of a level set function that is parameterized by radial basis functions, and the structural response is computed via the Interface-enriched Generalized Finite Element Method (IGFEM). Semi-circular cracks are assumed to nucleate at the location of enriched nodes that are crated throughout solid boundaries. Energy release rates (ERRs) for all cracks are evaluated by means of topological derivatives, for which we only require the stress field of a single finite element analysis of the uncracked geometry. To that end, an accurate nodal stress field is obtained by means of a non-local stress improvement procedure. The objective function of the topology optimization aggregates all ERRs using the P-mean function. Two schemes are proposed in relation to the direction of cracks: We first fix the crack opening direction to be parallel to either the xz or yz planes. We then relax this restriction and assume the crack opening direction to be perpendicular to the direction of the first principal stress. 3-D numerical examples, including the commonly studied L-bracket benchmark problem, showcase the capability of the procedure.

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TOPOLOGY OPTIMIZATION OF VIBRATING STRUCTURES AND PHONONIC CRYSTALS WITH PRESCRIBED FREQUENCY BANDS

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[2]Shandong University

ABSTRACT

Vibration brings lots of harmful effects for engineering structures in aerospace, high-speed train, and high precision machine, et. al. Thus, how to reduce structural vibration has been a hot topic in engineering and academics. For lots of engineering structures, such as machine tools, vibration isolators, et al., they usually work in some frequency bands[1,2]. When the working or external excitation frequency is equal to or close to the natural frequency of a structure, the resonance phenomenon will happen. Therefore, by reasonably designing the structures and adjusting the natural frequencies to keep away from the common manufacturing or working frequency bands can effectively mitigate the vibration level. In this study, a new continuous and differentiable mathematical formulation of the frequency band constraint[3] based on the modified Heaviside function is proposed to achieve the prescribed frequency bands of vibrating structures. Furthermore, compared to the vibration structural design, the difficulty of phononic crystals' prescribed frequency bands design lies in the correlation between stiffness matrix and wave vector, which is a typical multi-condition eigenvalue problem. Directly utilizing the frequency band constraints may lead to numerical convergence difficulties. Thus the ipsilateral frequency constraint based on a modified Heaviside function is further proposed. Since the developed functions are continuous and differentiable, the sensitivity of the constraint functions can be derived for using the gradient-based optimization solver. The proposed formulation can treat with multi-frequency band constraints and is easily integrated into a topology optimization model. Several numerical examples, including single- frequency band and double-frequency bands problems, are solved by the proposed method. The results validate the effectiveness of the developed method.

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Advanced model order reduction techniques for computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT AND ANALYSIS IN DATA-DRIVEN SYSTEM IDENTIFICATION METHODS WITH APPLICATIONS IN FLUID DYNAMICS

Xinyang Liu[*1]

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ABSTRACT

This work will focus on the development and analysis of data-driven system identification methods and applications in fluid dynamics. The objective is aiming to uncover the underlying pattern of the flow based on model-order reduction methods, in addition to the insights of the flow mechanics. The nature of fluid is very intricate mainly because of being nonlinear, immense in spatial-temporal dimensions, sensitive to the boundary conditions and it's interfered by the noise of irrelevant behaviors during the data measurement. The reduced-order models achieve to identify and reconstruct the principal dynamics indicating the physics of the respective flow. In addition, they filter the noise to prevent from the over-fitting problem. The understanding of the nature of fluid dynamics bridges from the broad existence to the numerous applications in diverse fields, such as performance improvement and energy saving in manufacturing which is a priority area in Canada.

Multiphysics biomechanics of bio- and bio-inspired soft materials: Theory, simulation and experiments
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A VISCO-HYPERELASTIC CONSTITUTIVE MODEL OF HYDROGEL BY CONSIDERING CHAIN'S SLIP MECHANISM

Qingsheng Yang[1] and Xinyu Liu[1]*

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ABSTRACT

Polymer is a typical entropic elastic material, and its mechanical response is highly decided by the change of network's conformation. The micro conformation's changing introduces the macro mechanical behavior. For finite deformation, the conformation changes not instantaneously, which leads to visco-hyperelasticity on macro. This process is not only related to loading time but also a multiscale question. In general, the conformation changes in two fields: 1) the single chain's deformation; 2) the relative position's change between chains. To build the bridge from micro to macro, a new transition is put forward in this work. The one-dimensional chain is extended to a three-dimensional cylinder to consider the effect of slippage. Another two free degree is introduced to capture the spatial-temporal characteristic of chain's conformation. The microscopic behavior of chain is then discussed and related to macro behavior of material. The slippage of chain is considered as the main reason leading to the viscosity by this model. This work provides an explanation for the origin of the viscosity in hydrogel by the opinion of chain's motion and gives a new method to build visco-hyperelastic constitutive model.

Advances in computational biomechanics and mechanobiology
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

OPTIMUM DESIGN METHOD FOR ARTIFICIAL EAR OSSICLES BASED ON A HIGH-PRECISION VIBRATION ANALYSIS MODEL

Yang Liu[1]*

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ABSTRACT

The conductive hearing loss occurs when the middle ear is damaged by various ear diseases, that results in hard sound conduction through the eardrum and three ossicles to the inner ear. The tympanoplasty operation is often carried out to reconstruct the damaged ossicular chain, and to improve the sound conduction efficiency. In the ossicular chain reconstruction, an artificial part called “columella” is produced and used instead of incus which is generally broken. In this operation, the sound conduction efficiency changes by the variations in the shape, material and mounting position of the columella. Currently, the operation is carried out based on the workmanship and experience of the surgeon. In our previous studies, dynamic characteristics of the middle ear in sound conduction have been investigated using three-dimensional finite element method. Based on the analysis results, we have proposed that the hearing restoration effect can be estimated by a comparison of the displacement of the steps footplate between a healthy model and an operation model. Then, designing a reasonable artificial auditory ossicle prior to the operation seems to become possible. However, most of these researches are confined to analytical research dealing with the effect of shapes or mounting positions of the columella, and the optimization based on numerical methods has not been studied.
In the present investigation, an intricate model for the analysis of middle ear vibrations with high precision was formulated, utilizing empirically obtained measurements. A finite element model was also established to simulate the operational dynamics of an impaired ossicular chain induced by chronic otitis media. Subsequently, topology optimization procedures were executed to systematically generate the most optimal configuration for the columella, a pivotal replacement component. The efficacy and soundness of the methodology advanced in this study were substantiated through rigorous verification processes. Notably, the topology optimization of the columella resulted in an augmented vertical displacement of the stapes baseplate, thereby exhibiting potential enhancements in auditory performance post-surgery.

Certification of simulations and model adaptation in computational science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GOAL-ORIENTED ADAPTIVE MULTILEVEL QUASI-MONTE CARLO FOR RANDOM ELLIPTIC PDES

Yang Liu[*1], Joakim Beck[1], Erik von Schwerin[1] and Raul Tempone[12]*

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[2]*RWTH Aachen University*

ABSTRACT

We present our work titled "Goal-oriented adaptive multilevel quasi-Monte Carlo (MLQMC) for elliptic random PDEs," building upon [Beck, Joakim, et al., "Goal-oriented adaptive finite element multilevel Monte Carlo with convergence rates." Computer Methods in Applied Mechanics and Engineering (2022)] and other ongoing research. Our objective is to solve an elliptic partial differential equation (PDE) with lognormal random input data, when the PDE model faces geometry-induced singularity.

Earlier research [Moon, K-S., et al. "Convergence rates for an adaptive dual weighted residual finite element algorithm." BIT Numerical Mathematics 46.2 (2006)] established convergence rates for a goal-oriented adaptive algorithm. This algorithm utilized isoparametric d-linear quadrilateral finite element approximations and the dual weighted residual error representation in a deterministic context. Notably, this algorithm refines the mesh based on the error's impact on the Quantity of Interest (QoI).

Our current work seeks to merge MLMC/MLQMC with the adaptive finite element solver. Unlike traditional Multilevel Monte Carlo methods, where each sample is determined using a discretization-based numerical method (with resolution tied to the level), our adaptive MLMC (AMLMC) algorithm employs a series of tolerances as its levels. Specifically, for a particular realization of the input coefficient and a set accuracy level, the AMLMC formulates its approximate sample using the initial mesh from the sequence of deterministic, non-uniform meshes. These meshes are produced by the previously mentioned adaptive algorithm and meet the sample-dependent bias constraint. Additionally, the incorporation of QMC enhances the convergence rate.

UQ-TTA student paper competition in uncertainty quantification
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GOAL-ORIENTED ADAPTIVE MULTILEVEL QUASI-MONTE CARLO FOR RANDOM ELLIPTIC PDES

Yang Liu[1], Joakim Beck[1], Erik von Scherwin[1] and Raul Tempone[1]*

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ABSTRACT

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A PHASE-FIELD APPROACH FOR THE NUCLEATION AND PROPAGATION OF DYNAMIC CRACKS

Yangyuanchen Liu[1], Oscar Lopez-Pamies[2] and John Dolbow[1]*

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ABSTRACT

Recently, Kumar et al. [1] proposed and revised a phase-field approach for the nucleation and propagation of fracture under arbitrary quasistatic loading conditions. The model accounts for an arbitrary material strength surface through an external driving force in the evolution equation for the phase-field. In this talk, we extend this model through the addition of inertial forces. The dynamic version of the model is then validated against a broad range of benchmark experiments for dynamic brittle fracture, including the experiments by Kalthoff and Winkler, the Brazilian fracture test, and a recent experiment investigating crack initiation, propagation and branching in soda-lime glass specimens [2]. Numerical simulations illustrate the proposed dynamic phase field model provides reasonable results compared to experimental observations and a cohesive phase field model by Geelen et al [3].

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Boundary element methods: New theories and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SOME ADVANCES ON THE FAST BEM FOR ACOUSTIC PROBLEMS

Yijun Liu[*1], Ruoyan Li[1], Zonglin Li[1] and Zhenyu Gao[1]*

[1]*Southern University of Science and Technology*

ABSTRACT

Some progresses on the boundary element method (BEM) for solving acoustic wave problems will be reported in this talk. For the frequency-domain acoustic wave problems, a new fast direct solver is proposed to improve the computational efficiencies in the solutions of the BEM equations. New enriched boundary elements based on the traditional constant elements and using plane wave expansions are also proposed to improve the representation of the variables on the boundary in the discretization of the boundary integral equations. For the 3-D time-domain acoustic wave problems, a new solution strategy based on the concept of a kernel-function library is developed in order to save the computer memory consumption in the solution of the time-domain BEM. Various examples using the above proposed new methods in the acoustic BEM are presented in this talk to show their accuracies and efficiencies in solving acoustic problems in both frequency and time domains.

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Recent advances on interfaces dynamics modeling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NEURAL NETWORKS WITH LOCAL CONVERGING INPUTS (NNLCI) FOR SOLVING CONSERVATION LAWS AND MAXWELL'S EQUATIONS IN VARYING DOMAINS WITH GREATLY REDUCED COMPLEXITY AND TRAINING COSTS

Harris Cobb[1], Haoxiang Huang[1], Hwi Lee[1], Yingjie Liu[1] and Vigor Yang[1]*

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ABSTRACT

This talk is based on a series of joint works (arXiv:2109.09316 and 2204.10424). With Haoxiang Huang and Vigor Yang, we are able to predict discontinuities and smooth parts of solutions of the Euler equations in 1D and 2D by a neural network accurately. For example, in order to predict the solution of the 1D Euler equations at a space-time location, one can design the output of a neural network to be the solution value at the location. If one tries to design the input as the low-cost numerical solution patch in a local domain of dependence of the location (where the information comes from), can the neural network tell if the input is across a shock or in a smooth region ? The answer is no! Our approach uses two numerical solutions of a conservation law from a converging sequence, computed from low-cost numerical schemes, and in a local domain of dependence of a space-time location as the input for a neural network to predict its high-fidelity solution at the location. Despite smeared input solutions, the output provides sharp approximations to solutions containing shocks and contact discontinuities. The method reduces the complexity by several orders of magnitude compared to a fine grid numerical simulation, has much lower cost to train, and can be used naturally in varying computational domains through training and prediction because it's a local method. It can be applied to other differential equations, e.g., the Maxwell's equations for solving electromagnetic waves scattered around complicated PECs (Cobb, Lee and Liu, arXiv:2302.02860).

Multi-scale and machine learning-based modeling methods for optimization and design of composites
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GENERATIVE MODEL TO PREDICT THE DEFORMATION FIELD OF CFRP LAMINATES WITH GEOMETRIC DEVIATIONS IN WING ASSEMBLY

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ABSTRACT

Thin-walled structure of CFRP laminates is widely utilized in the assembly of aircraft wings. The deformation field generated during the assembly process can impact the assembly performance of the structure, thereby influencing the product quality and operational performance of the wings. The geometric deviations on the critical mating surfaces of the laminate are key factors influencing the deformation fields during the assembly process. Analyzing the mapping relationship between geometric deviations and assembly deformation field plays a crucial role for assessing the assembly results. The traditional analysis methods only consider the impact of simple directional deviations on assembly results and do not comprehensively account for the part geometric deviations. This paper proposes a deviation- deformation analysis framework for CFRP laminates in aircraft wing assembly. The framework introduces a multi-scale geometric deviations modelling method based on the statistical parameters for critical assembly features. Subsequently, it integrates heterogeneous data characterizing shape deviations by employing the encoders. Finite element analysis is then conducted to calculate the assembly deformation field considering the constitutive relationships and damage mechanisms. Taking the parameters representing the geometric deviations as input and deformation field as output, a conditional generative model is employed to learn the influence pattern of the geometric deviations on the deformation field. The framework establishes a prediction model from the deviation field to the deformation field and introduces specific accuracy metrics. Corresponding simulations and experiments demonstrate that the proposed method can predict assembly deformation field more efficiently than traditional numerical methods. It exhibits excellent performance on the accuracy metrics, enabling accurate and efficient field-to-field predictions. This method, by learning expert knowledge such as damage mechanisms and mechanical characteristics during the assembly process, constructs an end-to-end deformation prediction for the CFRP laminates. The predicted results can serve as a research framework for predicting other physical fields.

Machine learning and data driven based engineering computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ANISOTROPIC TAILORED SPINODOID MECHANICAL METAMATERIALS: CONSTITUTIVE MODEL-GUIDED RAPID INVERSE DESIGN AND APPLICATION IN ARTIFICIAL BONE IMPLANTS

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ABSTRACT

Spinodoid mechanical metamaterials have garnered significant attention in designing lightweight, high-strength engineering structures and medical implants due to its tunable extreme anisotropic behavior. However, the lack of explicit relationship between complex topology and anisotropic mechanical properties severely restricts rapid inverse design and metal additive manufacturing for spinodoid materials with desired mechanical response. In this study, an integrated methodology leveraging constitutive model-guided rapid inverse design and additive manufacturing for spinodoid metamaterials is developed. First, the volume-fraction- and fabric-tensor-based orthotropic constitutive model for spinodoid materials is developed to describe how topological parameters determine effective mechanical properties. Guided by the parametric constitutive model, representative spinodoid structures are efficiently selected to characterize the mechanical property variation in the whole material space. Next, a deep learning-based model trained by 256 representative spinodoid samples is proposed to inversely design tailored spinodoid materials, which substantially reduces the training sample demand and promotes the pretraining efficiency of design model. Furthermore, by representing the complex 3D spinodoid structure as a two-dimensional topological parameter via dimension reduction method, the explicit structure-property relationship for arbitrary topological parameters is built and the target structure can be efficiently searched by a global optimization strategy. At last, the approach is successfully applied in metal additive manufacturing for tailored spinodoid materials with Ti6Al4V that matches the orthotropic mechanical properties of cancellous bones. The new approach paves an efficient way to build the property-structure-process relationship for precision-engineered spinodoid mechanical metamaterials with tailored mechanical performance in various applications.

Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STABILIZED UNFITTED FINITE ELEMENT METHOD FOR HYDRO-MECHANICAL COUPLING WITH WEAK DISCONTINUITY

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ABSTRACT

The traditional finite element method requires that the mesh must match with various discontinuous, which can significantly increase the difficulty of preprocessing for hydrodynamic coupling problems with complex boundaries and material interfaces. In such case, the finite element method using unfitted mesh is obviously more advantageous, however, this method also has certain problems, for example, irregular mesh cutting may lead to ill-conditioned coefficient matrix to appear, which in turn affects the accuracy and stability of the algorithm. The ghost penalty technique was proposed to overcome the ill-conditioning issue. Recently, an unfitted finite element was proposed for two-field poroelasticity problem, where stabilization terms based on the ghost penalty were developed. Material interfaces are even more difficult to deal with than the boundary as they require careful treatment of the weak discontinuity conditions as well as the mesh cutting stabilization. In this paper, we formulate an unfitted finite element for the poroelastic problem with both material interfaces and complex boundaries. A weak formulation based on the Nitsche's method was developed. Ghost penalty stabilization terms are designed for both sides of the elements intersected by the material interface. The performance of the proposed methodology is tested by several benchmark and practical hydraulic problems of complicated rock-soil mixtures. The numerical results demonstrate optimal convergence rates and low-level condition numbers independent of the mesh cutting.

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Uncertainty quantification and reliability analysis in engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DIMENSION-REDUCTION REPRESENTATION FOR STOCHASTIC GROUND MOTIONS AND ENGINEERING APPLICATIONS

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ABSTRACT

When using frequency domain analysis methods to simulate random seismic actions, both traditional spectral representation and proper orthogonal decomposition belong to the conventional Monte Carlo simulation method. Currently, the conventional Monte Carlo simulation method still face difficulties such as large random variable dimensions, low accuracy of finite simulation samples, and random convergence. To solve these difficulties, this study first derives the original spectral representation (decomposition) of non-stationary random (vector) processes, The sources and significance of classical random amplitude method and random phase method are provided. On this basis, a dimension-reduction representation based on random orthogonal functions is further proposed, which introduces the constraint form of random orthogonal functions to accurately express the full probability information of the random (vector) processes of seismic ground motions with merely several elementary random variables. This dimension-reduction representation has achieved simulation of non-stationary ground motion processes, multi-point and multi-dimensional ground motion vector processes, and continuous ground motion fields. Benefitting from the dimension-reduction representation, each representative sample has assigned probability and all the probabilities constitute a complete set, which lays a solid foundation for the refined analysis of non-linear seismic response and dynamic reliability of engineering structures within the third structural design theory. By far, the dimension-reduction simulation method has been successfully applied to the stochastic dynamic response and overall reliability refinement evaluation of complex engineering structures such as high-rise buildings, large-span bridges, and dams under earthquake action.

Computational mechanics in Canada and China: Current states of shared scientific interests and opportunities for the future cooperation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT AND ANALYSIS OF THE THEORY OF COMPOSITE EXPANSION RING UNDER ELECTROMAGNETIC LOADING

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ABSTRACT

High-speed impact collisions are common mechanical problems in engineering and life. Researchers have recognized that the response of objects under impact loads significantly differs from that under static loads. The dynamic mechanical parameters of materials are crucial for predicting their mechanical response under dynamic loads. Electromagnetic loading expansion ring test technology is essential to achieving a high strain rate tensile loading of materials. The intense pulse Lorentz force is sufficient for low resistivity specimens to achieve the desired strain rate. However, for high resistivity specimens, the induced current is relatively small under achievable loading voltages, making it challenging to obtain satisfactory loading results. Using a low resistivity pusher, the composite expansion ring loading scheme promotes specimen expansion and enables electromagnetic loading expansion ring tests to achieve dynamic tensile loading on most materials. Nevertheless, since this proposed test method, the theory of electromagnetic loading composite expansion rings has yet to develop fully.

This paper comprehensively analyzes the dynamic induction of coil, pusher, and specimen during the process where the pusher promotes the specimen's expansion. It considers the influence of electromagnetic-thermal-mechanical coupling on load results during electromagnetic loading processes and proposes a compound theory capable of accurately predicting composite expansion ring load processes. The simplified compound theory is also presented when dealing with specimens with relatively large resistivities.

The proposed theories in this paper are validated through numerical simulation methods. Furthermore, this paper analyzes the impact of driving ring materials on electromagnetic loading results and investigates how parameters such as coil and capacitance affect electromagnetic loading outcomes. Finally, the applicability of the simplified compound theory is discussed. This paper provides theoretical support for the design of the composite expansion ring under electromagnetic loading.

Constitutive modeling of complex materials with machine learning and artificial intelligence
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VARIATIONAL SYSTEM INFERENCE OF PHASE FIELD FRACTURE MODELS

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ABSTRACT

The mechanical behavior of biological materials is systematically studied in the paradigm of continuum mechanics. Complex phenomena, such as damage and fracture, have been modeled using the phase-field framework in which the total energy functional is minimized with respect to the deformation fields and internal variables (i.e. phase fields) to determine the material's mechanical response [1]. This approach is popular since it can model crack nucleation, propagation, branching, and merging without the need for distinct methods or additional discontinuities in the solution fields. In this work, we present a data-driven inverse method to infer the parameters of a phase-field model of fracture for materials exhibiting complex mechanical responses.

The phase-field fracture formulation has been applied in challenging biological applications such as angioplasty, aneurysm, and ligament tears [2]. This model utilizes hyperelastic free energy that degrades with evolving phase field to model damage and fracture in biological tissues. This general framework takes a modular approach to select a nonlinear stress-strain response and fracture dynamics from a set of hyperelastic models and fracture growth laws, respectively. In our data-driven approach, we identify the best hyperelastic free energy form and damage growth laws from a set of admissible candidates.

We formulate an algebraic optimization problem by considering the weak form of the momentum balance equation with different constitutive models and apply it to the deformation fields. We infer the parameters in the constitutive model and sequentially drop the non-contributing terms to infer the best-suited parsimonious model. This approach is referred to as Variational System Identification [3]. We demonstrate the performance of our methods in the face of noisy data that challenges the identification of mathematical models while attaining high accuracy in the predicted response of the inferred models.

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COMPUTATIONAL MODELING OF MULTILAYERED BENDING PLATES (A 2D+ MULTISCALE APPROACH)

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ABSTRACT

This study introduces a novel 2D multiscale strategy, referred to as the 2D+ approach, employing a computational homogenization formalism tailored for modeling multilayered plates in situations dominated by bending. Such structural elements often involve advanced materials like laminated composites, characterized by a heterogeneous distribution of low-aspect-ratio layers exhibiting substantial nonlinear mechanical behavior across their thickness.

In this methodology, the macroscopic scale is represented by the 2D plate mid-plane, while the mesoscopic scale employs a 1D filament-like Representative Volume Element (RVE) orthogonal to the plate mid-plane, spanning the plate thickness. This RVE captures nonlinear mechanical behavior across the plate thickness at each integration point of the 2D plate discretization. The selected kinematics and discretization at these scales are chosen to effectively capture nonlinear mechanical behavior, achieve computational efficiency, and provide accurate stress distributions compared to high-fidelity 3D simulations.

The proposed strategy aligns with the standard first-order hierarchical multiscale framework, involving the linearization of the macro-scale displacement field along the thickness. It incorporates an additional fluctuating displacement field in the RVE to capture higher-order behavior, computed through a local 1D finite element solution of a Boundary Value Problem (BVP) at the RVE.
A notable feature of the 2D+ approach is the application of the Hill-Mandel principle, establishing mechanical energy equivalence in both macro and meso scales. This weakly couples the 2D macroscopic plate and the set of 1D mesoscopic filaments, resulting in significant computational savings compared to standard 3D modeling. Solving the resulting RVE problem in terms of the fluctuating displacement field enables the enforcement of an additional condition: the fulfillment of linear momentum balance (equilibrium equations). This yields a physically meaningful 2D-like computational setting for the considered structural object (multilayered plates under bending), providing accurate stress distributions typical of full 3D models at the computational cost of 2D models.

DEVELOPMENT, VERIFICATION AND VALIDATION OF 3D FEA-BASED SURROGATE MODELS FOR DAMAGE TOLERANCE APPLICATIONS

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ABSTRACT

The two requirements for a cost-effective modeling procedure in probabilistic fatigue crack growth life assessment are solution accuracy and runtime speed. Quite often, solution accuracy is sacrificed for computational cost using reduced-order models, which can carry some level of solution uncertainty. To overcome such shortcomings, a 3D Finite Element (FE) modeling procedure capable of inserting, analyzing and propagating arbitrary-shaped cracks is employed to generate accurate solutions without the simplifications of geometry, crack shape/path and loading which are associated with reduced-order models.

Since 3D FEM solutions tend to be computationally expensive, machine learning algorithms (surrogate modeling) are used here to leverage the accuracy of the 3D FEM and reduce runtime. Depending on the type of the life assessment requirements, the deterministic solutions consisting of stress intensity factor values, remaining useful life or a 3D crack propagation path, are used for calibrating the surrogate models. The 3D FEA-based surrogate modeling allows for the parametrization of the geometry of interest, loading conditions, crack location, and can be further utilized in probabilistic life assessments. For instance, it can account for intrinsic fatigue crack growth rate scatter as a source of material behavior uncertainty.

Two types of surrogate models suitable for use in probabilistic fatigue crack growth life assessment are developed. For mode I applications, Gaussian Process Regression (GPR) is employed, while for mixed-mode loading cases, where the out-of-plane crack path is a critical output, Radial Basis Function (RBF)-based response surface modeling is utilized. A 3D finite element modeling procedure is used to generate accurate solutions to train the surrogate models, and verification is performed on both types of calibrated surrogate models. Experimental measurements are used to provide validation references for deterministic as well as surrogate modeling solutions.

It was demonstrated that the two surrogate modeling types (GPR and RBF response surface) significantly reduce the solution runtime compared to their deterministic counterparts, making them suitable for probabilistic damage tolerance assessments.

Computational damage and fracture mechanics
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IMPLEMENTATION OF MICRO-MECHANICAL MODELS FOR MICRO-STRUCTURAL BASED CHARACTERIZATION OF COHESIVE ZONE MODELING (CZM) PARAMETERS FOR DIFFUSION BONDED COMPONENTS

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ABSTRACT

Multilayered aluminum components are of great interest in the aerospace industry due to their high strength-to-weight ratio and corrosion resistance. One of the common production methods of such layered components is diffusion bonding of similar and dissimilar metals. For load bearing applications the bond strength between the different layers is critical. Alongside experimental techniques for assessing bond strength in layered components, a computationally efficient method to model interface failure is the cohesive zone approach (CZM). In this framework the mechanical response of the interface is governed by a traction-separation law (TSL). The TSL represents the relation between the stresses across the interface and the relative displacement between layers, capturing the loss of load-bearing capacity before the final layer separation.

The TSL parameters are commonly determined by fitting of experimental load displacement data and numerical simulations (FEM). In such an approach, micromechanical aspects such as bonding defects (micro-voids) due to oxide layer fracture along the interface, which are known to greatly influence the bond strength, cannot be directly taken into consideration. The goal of the current study is to utilize a micromechanical based FE approach in conjunction with a Continuum Damage Model (CDM) approach to determine the TSL parameters, of diffusively bonded aluminum 7075 specimens, solely based on the defects pattern observed at the interface and a ductile failure law for Al 7075. First the flow-stress of Al7075 at temperatures of 400-500C was determined by cylindrical compression experiments and finite element modelling. Next, Al7075-Al7075 specimen pairs underwent diffusion bonding at 400-500C and thermo-mechanical finite element modelling was used to compute the time dependent thermo-mechanical fields at the specimen interface. Following the bonding experiments, small tensile specimens were cut from the bonded pairs and underwent characterization of the interface using a Scanning Electron Microscope (SEM) and subsequent mechanical testing. The, interfacial morphology observed from the SEM imaging was used to construct microstructural based Representative Area Elements (RAE) of the interface area. To model intact bond failure of the Al7075 in the RAE, a continuum damage approach for Al7075 previously published by the authors was utilized [1]. It is demonstrated that effective TSL can be obtained from the micromechanical models which explicitly take micro-structural parameters of the interface into consideration.

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Current trends in phase-field modeling and computations
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AN EXTENDED PHASE-FIELD METHOD FOR FRACTURE SIMULATIONS

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ABSTRACT

The extended phase-field method (XPFM) combines the phase-field method for fracture with concepts from the extended/generalized finite element method. The approach aims at a significant reduction of the computational effort in comparison to the standard phase-field method while keeping the advantages of not having to explicitly track the crack geometry and to introduce additional crack propagation criteria.

The XPFM is based on a transformed phase-field ansatz and an enrichment of the displacement field. This allows for much coarser meshes, and it leads to truely mesh independent crack geometries including cracks that run through elements. The transformed phase-field ansatz incorporates knowledge about the analytical solution of the phase-field equation in 1D. The displacement enrichment is entirely based on the phase-field solution, and in contrast to the initial XPFM approach [1], in the present, refined version of the XPFM the necessity to calculate the direction perpendicular to the crack can be avoided completely. This allows for more general applications and the extension of the XPFM to 3D. The displacement enrichment is computed in a discrete way on a subgrid within each enriched finite element on which a phase-field dependent Laplacian problem needs to be solved for each direction. The respective scalar solution fields for the discrete displacement enrichment functions can be obtained in a very efficient way.

In this contribution, the latest developments for the XPFM including the algorithmic treatment will be presented, and applications to common academic examples for the simulation of fracture processes will be shown.

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Modeling, simulation, and AI for ultrasonic NDT and SHM
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NOVEL VARIATIONAL AUTOENCODER ARCHITECTURE FOR TEMPERATURE-ADAPTIVE ULTRASONIC GUIDED WAVE GENERATION

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ABSTRACT

Ultrasonic guided waves (UGWs) have recently captured the attention of the structural health monitoring (SHM) community. This heightened interest primarily stems from the remarkable sensitivity of UGWs to alterations in the properties of the medium through which they propagate. This makes such waves an interesting diagnostic tool to identify and describe damage affecting thin-walled structures. Among the results of damage diagnosis procedures, anomaly localization is fundamental to drive maintenance actions and restore the health state of the structure. To date, localization has predominantly relied on tomographic algorithms. Despite being widely adopted, they come with unsolved issues, including the generation of artifacts in damage probability maps and the bad performance under varying environmental and operational conditions (EOCs). Consequently, supervised data-driven approaches for UGW-based damage diagnosis have been proposed in the literature. Although such methods are characterized by satisfactory performance, a notable constraint is the requirement for large high-fidelity datasets for training the algorithms, which are typically unavailable for real-life structures. Furthermore, such methods still cannot deal with varying EOCs. A potential remedy lies in unsupervised machine learning methods. These methods have already found application in damage detection within the SHM field, but unsupervised approaches that can localize damage under varying EOCs still have to be investigated in detail. This work aims to overcome the limitations mentioned above by proposing a novel unsupervised network architecture based on variational autoencoders (VAEs). The algorithm was trained over an experimental dataset of UGWs acquired under varying temperature conditions. Testing was performed against experimental signals acquired at temperatures not seen during training to verify that the generative artificial intelligence tool is able to capture the influence of temperature on UGWs.

Computational damage and fracture mechanics
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COHESIVE XFEM FORMULATION FOR DUCTILE FRACTURE AT LARGE DEFORMATION

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ABSTRACT

Numerical simulation aided design of large-scale metal and alloy structures under extreme conditions, such as accidental mechanical overloads that may lead to failure, remains a major concern of various industrial sectors such as transportation, energy, and defense.

In this work, we present a three-dimensional numerical approach able to macroscopically account for various dissipative mechanisms (e.g., plasticity and ductile damage) leading to failure. The methodology is developed within the finite strain framework and is implemented into ABAQUS-std finite element computational code as a user finite element (UEL), in view of ensuring mesh-objective results.

Key features of the methodology include its treatment of both geometric and material nonlinearities using an updated Lagrangian formulation (ULF) [1]. The phase of more or less diffuse damage is reproduced by using Gurson-Tvergaard-Needleman (GTN) microporous plasticity model [2] employing standard finite element methods (FEM). Furthermore, the micro-void coalescence phase-induced dilation/shear band is modeled using an innovative extended cohesive finite element approach (XFEM-CZM) [3]. The progressive loss of cohesion culminating in ultimate cracking is addressed with the extended finite elements method (XFEM). A particular attention is paid to transition criteria (damage to localization, localization to cracking), the orientation of the localization plane (especially in Mode II), the cohesive zone model (empirical vs. inspired by the micromechanics of micro-void coalescence), and techniques for overcoming numerical challenges (e.g., volumetric locking [4], numerical integration [5]).

The unified methodology is shown to be able to replicate the degradation process until fracture (progressive drop in resistance, fracture surface orientation) in large elastoplastic deformation of structures used in laboratory tests, even with relatively coarse meshes.

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Contact and interface mechanics: Modeling and computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING SOLID-SOLID CONTACT IN A FULLY EULERIAN PHASE-FIELD FRAMEWORK

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ABSTRACT

This work introduces a novel Eulerian finite element framework based on a phase-field representation of solids to model mechanical contact between elastic solids, with a particular focus on systems involving evolving and intricate surfaces [1]. Traditionally, Lagrangian frameworks dominate in modeling such interactions, yet they often demand sophisticated algorithms for contact detection and resolution. Furthermore, they face difficulties when dealing with solids undergoing dynamic boundary changes, such as crystals growing within confined spaces. Because the physical or chemical evolution demands an Eulerian framework, it is desirable to phrase the mechanical solid boundary value problem in such a framework as well, requiring novel approaches to contact modeling.

Our approach employs the phase-field method that includes a diffuse representation of geometries on a spatial mesh, streamlining the modeling of evolving surfaces. To model elasticity, we make use of the reference map technique [2]. A distinctive feature of our methodology is the introduction of volumetric penalty forces that weakly enforce the contact constraint. Capitalizing on the single reference system, the traction force is defined as a simple function of the phase-fields of the two bodies in contact, which renders contact search obsolete. We demonstrate the validity and versatility of our method through numerical examples, showcasing its capability to accurately capture complex solid-solid interactions.

The Eulerian phase-field formulation significantly simplifies the complexities associated with contact detection and resolution in traditional Lagrangian contact models. Additionally, our framework can be used to seamlessly integrate with other physical phenomena by incorporating multiple energy terms in the evolution of the phase-field. This enables the modeling of multiphysics scenarios, presenting a valuable tool for a broad spectrum of applications involving chemically or physically evolving deformable solids in contact. Such scenarios are, for example, prevalent in deterioration processes of porous media.

In conclusion, our Eulerian finite element framework provides an innovative and promising alternative solution for modeling contact between elastic solids, particularly in scenarios with evolving and intricate surfaces. The methodology's adaptability and capability for multiphysics modeling makes it a promising tool for addressing a wide range of applications, offering insights into the mechanical interactions of deformable solids in contact during processes like growing corrosion precipitates in porous media.

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REDUCED ORDER MODELLING OF EXACT PERIODIC FLOWS USING A SPACE-TIME DISCRETISATION

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ABSTRACT

Periodic flows are omnipresent in a large number of industrial applications. Examples include the flow past wind turbines, rotating flows in turbomachines and the pulsatile flow of blood. Simulation of periodic flows is computationally demanding for design and control applications as they need a long time domain for periodicity in the flow to develop. We circumvent the problem by using a parametric POD-Galerkin reduced order model, which exploits the nature of the problem.

In the full-order model, we apply the framework of residual-based variational-multiscale turbulence modelling and space-time iso-geometric analysis to solve the incompressible Navier-Stokes equations [1]. We convert the initial value problem to a boundary value problem by applying a periodic boundary condition in time to compute the time-periodic states directly. We use the Proper Orthogonal Decomposition (POD) to create a basis using parameter-dependent solutions from the full-order model. The time-periodic basis contains information on space and time, allowing for a dimension reduction in both. We create the reduced-order model using the POD basis and the same stabilisation as the full-order model [2,3]. The reduced-order model can use the DEIM, Q-DEIM and the S-OPT hyper-reduction techniques.

We apply the reduced-order model to flow past periodically heaving and pitching hydrofoils at a Reynolds number of O (103). Parameters include heave amplitude and motion period. The numerical experiments show a fast decay in singular values, allowing for small basis sizes. The results are in agreement with the results of the full-order model.

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Computational models and methods for predicting cancer progression and treatment response
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STRATEGIC INTEGRATION OF PREDICTIVE MODELS: A HOLISTIC APPROACH TO DECIPHERING BREAST CANCER METASTASIS DYNAMICS

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ABSTRACT

In recent years, transformative technological advancements have markedly enhanced our ability to detect individual cancer cells and clusters within patients' blood, lymph nodes, and bone marrow. Despite these groundbreaking developments, the clinical significance of these detected cells remains elusive. This study addresses this uncertainty by introducing a systematic framework designed to select hypotheses that elucidate the population-level dynamics of non- and post-hypoxic cells during breast cancer metastasis to lung tissue. This framework leverages rich data obtained from meticulously conducted ex vivo experiments. Additionally, our approach employs an agent-based model, strategically translating macroscopic information into a microscopic perspective. This enables a comprehensive exploration of dynamic processes and facilitates the generation of novel hypotheses regarding breast cancer metastasis. The efficacy of our framework is demonstrated through the rigorous testing of 1152 candidate models at the population level, resulting in the efficient elimination of unlikely hypotheses and the revelation of valuable insights into the intricate metastatic process. Our multiscale model intricately unravels the proliferative advantage held by non-hypoxic cells within the lung tissue microenvironment. These findings contribute significantly to a deeper understanding of breast cancer metastasis dynamics and bear implications for the development of future therapeutic interventions. This integrated approach serves as a bridge between recent technological breakthroughs and sophisticated modeling techniques, thereby advancing our collective understanding of the complexities inherent in breast cancer metastasis.

Data-enhanced multi-model uncertainty quantification and experimental design of complex computational systems
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A MULTI-FIDELITY APPROACH TO PREDICTION OF FLUTTER BOUNDARY UNDER UNCERTAINTY

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ABSTRACT

We present a multi-fidelity uncertainty quantification (UQ) approach that leverages multiple computational aeroelasticity (CAE) models of various accuracies and costs to characterize the flutter boundary of a wing under uncertainties. The accurate determination of the flutter boundary, which corresponds to the point where the aeroelastic system exhibits zero damping and indicates the onset catastrophic unbounded oscillation, is crucial to aircraft certification. In the presence of model parameter uncertainties, aircraft may experience flutter far below the predicted flutter speed [1]. Our goal is to quantify this uncertainty and to provide the probability of flutter for a range of flight conditions. The problem can be considered a probabilistic extension of the deterministic flutter prediction using multi-fidelity models considered in [2]. Our multi-fidelity UQ approach builds on the following three ingredients: Gaussian process models, which readily incorporate sampled responses from models of various fidelities and provide probabilistic estimates of the damping coefficient over the parameter space; an input-dependent error estimate throughout the parameter space for each model, which is constructed by appealing to the predicted model discrepancies across levels of model fidelities; and contour-targeting adaptive sampling strategies, guided by the expected improvement in and/or estimates of approximation error, to select a sequence of models and sampling points that best improves the approximation of the flutter boundary while accounting for model evaluation costs. We demonstrate the multi-fidelity method for a transonic flutter problem using the following models: a Reynolds-averaged Navier-Stokes CAE model; a Euler CAE; and a traditional aeroelasticity model based on Theodorsen's aerodynamics. The multi-fidelity method enables efficient characterization of the probabilistic flutter boundary and accurately captures the sharp decrease in flutter velocity in the unsteady transonic flow regime with proper model selection.

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EMULATING OCEAN MODELS TO QUANTIFY UNCERTAIN RESPONSES TO CLIMATE CHANGE

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ABSTRACT

To better understand the responses of ocean systems to different forcings that represent climate change scenarios, we have explored a wide range of values for the parameters and initial/boundary conditions in an idealized ocean model on a global scale, NeverWorld2, which has intermediate complexity: it incorporates basin-scale geometry for an idealized Atlantic and Southern ocean, with non-uniform ocean depth to allow for mesoscale eddy interactions with topography. The simulation is implemented in Oceananigans.jl, a Julia-based software package for finite volume simulations of the nonhydrostatic Boussinesq equations on CPUs and GPUs. Due to the complexity of global circulation models, however, simulations of ocean processes are prohibitively expensive (even on GPUs), making the tasks of uncertainty quantification for future predictions and sensitivity analysis for model parameters extremely challenging. To address this challenge, we have investigated a wide range of deep learning tools to build dynamical emulators for targeted quantities of interest (QoIs). In addition, we have explored and developed systematic ways of identifying additional informative or dynamically relevant variables from the governing system, to make these QoI emulators more predictive and accurate. The efficient emulators will make it possible to capture interactions between the ocean and other components of climate models (e.g., atmospheric models, land models, human activities). This provides valuable scientific information for stakeholders in fighting climate change.

The phase field method for fracture: Theory, numerics, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A GENERALIZED FRAMEWORK SUITABLE FOR DYNAMIC AND ELASTIC-PLASTIC CRACK GROWTH PROBLEMS: THE PRINCIPLE OF LEAST EXTERNAL WORK

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ABSTRACT

Starting from the principle of least action, we propose the principle of least external work suitable for dynamic and elastic-plastic crack growth problems. Among those possible crack growth patterns, the principle of least external work indicates that the real one consumes the minimum value of the external work. Like the phase-field method, the proposed principle also converts crack growth problems into an energy minimization value problem, except that the energy term here is the work applied by external loadings. According to the first law of thermodynamics, external work can convert into kinetic energy, elastic and plastic deformation energy, or fracture energy. Therefore, the proposed principle can naturally apply to dynamic and elastoplastic crack growth problems.

Moreover, it can be proved that:
1) For the pure deformation of an elastic solid, the principle of least external work is equivalent to the principle of minimum potential energy;
2) In the case of quasi-static crack growth in elastic solids, the principle of least external work can give the Griffith criterion [1];
3)When a crack grows dynamically in an elastic solid, the principle of least external work can derive the dynamic fracture criterion proposed by Freund [2];
4) When a crack propagates quasi-statically in an elastic-plastic solid, the principle of least external work will give the fracture criterion based on the incremental J-integral [3].

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Battery modeling and computation: From material to device
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTI-PHYSICS SIMULATIONS FOR LI BATTERY

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ABSTRACT

In this talk, I will present some of our recent work of developing battery simulation tools, and how these tools may help facilitate the battery design and management. The prediction of capacity fade and lifetime of batteries is important for cell design, determination of the optimal operation condition and control, and cell maintenance. Various mechanisms contribute to capacity fade. I will talk about a comprehensive capacity fade model and its experimental validation and application for battery optimization; a multiscale approach that couples mechanics and electrochemistry consistently at both particle and electrode scales which enables simulating various electrode phenomena; and approaches to optimize battery health while fulfilling both energy and power requirements. In simulation-based battery design, a large amount of simulations are required to determine the optimal design variables. The computational cost can be prohibitively expensive. I will introduce a new approach of Self-directed Online Learning Optimization (SOLO), which integrates dynamic deep neural network with finite element calculations. SOLO reduces the computational time by up to 5 orders of magnitude compared with directly using heuristic methods, and outperformed all state-of-the-art algorithms tested in our experiments. I will also show a pruner and sampler approach to determine model parameters or battery design parameters, which can reduce the battery testing time by about 75%. Finally, I will discuss simulations of concurrent dendrite and SEI growth.

Battery modeling and computation: From material to device
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

REACTIVE DIFFUSION OF LITHIUM IN SILICON – NEW INSIGHT FROM ATOMISTIC SIMULATIONS

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ABSTRACT

Atomistic simulations are performed to investigate the insertion of lithium (Li) in crystalline silicon (c-Si) by using a modified embedded atom method potential. The mechanism for the formation of the amorphous a-LixSi was analyzed by conducting novel structural analysis. Diffusion pathways of Li in c-Si and the energy barrier are also analyzed and calculated. The results show that Li atoms diffuse preferably along the 112 directions on the {111} planes, and the energy barrier is too high for thermally activated diffusion around room temperature. The formation mechanism for the amorphous/crystalline interface (ACI) is also analyzed. The diffusivity of Li in Si is calculated based on the simulation results. Our results show that the diffusivity of Li in the a-LixSi is about 50~100 times faster than in the c-Si. Our results also show that the composition of Li in the a-LixSi is non-uniform during lithiation, and the distribution of Li is analyzed. The simulation results are compared with the available experimental results.

The phase field method for fracture: Theory, numerics, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STABILIZED FORMULATION FOR PHASE-FIELD FRACTURE IN NEARLY INCOMPRESSIBLE HYPERELASTICITY

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ABSTRACT

This work presents a stabilized formulation for phase-field fracture of hyperelastic materials near the limit of incompressibility. At this limit, traditional mixed displacement and pressure formulations must satisfy the inf-sup condition for solution stability. The mixed formulation coupled with the damage field can lead to an inhibition of crack opening as volumetric changes are severely penalized effectively creating a pressure-bubble. To overcome this bottleneck, we utilize a mixed formulation with a perturbed Lagrangian formulation which enforces the incompressibility constraint in the undamaged material and reduces the pressure effect in the damaged material. A mesh-dependent stabilization technique based on the residuals of the Euler–Lagrange equations multiplied with a differential operator acting on the weight space is used, allowing for linear interpolation of all field variables of the elastic subproblem. This formulation was validated with three examples at finite deformations: a plane-stress pure-shear test, a two-dimensional geometry in plane-stress, and a three-dimensional notched sample. In the last example, we incorporate a hybrid formulation with an additive strain energy decomposition to account for different behaviors in tension and compression. The results show close agreement with analytical solutions for crack tip opening displacements and performs well at the limit of incompressibility.

Multiscale modeling, analysis and numerical methods of material defect and inhomogeneities
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL SIMULATION OF MATERIAL STRENGTH OF CMCS BASED ON CT DATA RECONSTRUCTION

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ABSTRACT

Ceramic-Matrix-Composites are an important material candidate for thermal structures in aero engines. To investigate the strength failure of CMC materials occurring at ordinary temperature service, this paper establishes a detailed geometric model of the material by obtaining the material structure and defect distribution characteristics through CT technology and establishes a strength prediction model of ceramic matrix composites at ordinary temperature by writing different material subroutines for the failure modes of different kinds of materials.

First, we carried out the geometric analysis model and FEM model construction for 2D-C/SiC composites containing defects. Using μX-CT technique, we conducted CT scans on four specimens of 2D-C/SiC composites at different locations and sizes, respectively. Based on the CT slice data obtained from the scans, the volume fraction and location distribution of defects were obtained by reconstructing and analyzing the material defects. Meanwhile, by analyzing the CT slice data, we obtained the geometric parameters of fiber bundles in 2D-C/SiC composites, characterized the geometry of fiber bundles more accurately, and placed the hole-type defects completed by the analysis into them, and finally obtained the single-layer finite element analysis model of 2D-C/SiC composites and the structural FEM of 2D-C/SiC composites.

Next, numerical simulations of the strength of 2D-C/SiC composites were performed. Based on FEM, the fiber bundles consisting of fibers and matrix are equated to a homogeneous material by the known use of the equivalent homogenization method. By writing the VUMAT subroutine, we defined the fiber bundle failure criterion and the matrix failure criterion respectively, and simulated the static tensile process of the material. In the simulation, we found that during the static stretching of the material, the damage of the material occurs first below the location of the coating cracks, and the cracks gradually expand downward with the increasing tensile load. After the failure of the first layer, the crack expansion path changed clearly from directly below the coating crack defect to the maximum bending position of the woven structure, which is more in line with the crack expansion law of CMC material in the static tensioning process. Through the numerical simulation analysis of the static tensile strength of the material at room temperature, the tensile strength of the material at room temperature was determined, and the reliability of the finite element model was also verified by combining the test results. This supports the effective data for ceramic matrix composites in material design and engineering applications.

Uncertainty quantification and reliability analysis in engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RELIABILITY ANALYSIS OF CABLE-STAYED BRIDGE SYSTEM BASED ON DIRECT PROBABILITY INTEGRAL METHOD

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ABSTRACT

The system reliability analysis of cable-stayed bridges is an important part of structural safety analysis, and this paper proposes a method to analyze the overall dynamic reliability of prestressed concrete cable-stayed bridges based on the direct probability integral method. Firstly, the limit state equations of the main girder bending strength failure, wind-induced vibration failure and the main tower strength damage failure in the downward direction and the transverse direction buckling failure as well as the strength damage failure of the tie ropes of the cable-stayed bridge are established. Then the reliability analysis of the whole bridge cables is carried out, and the most dangerous three pairs of cables are selected to form a series-parallel system with the failure modes of the main girders and towers of the cable-stayed bridge, and the joint probability density integral equations of the extreme value mapping of multiple performance functions are established. Finally, the equations are solved using the direct probability integration method containing Heaviside function (DPIM-H) to obtain the overall dynamic reliability index of the cable-stayed bridge, and the Monte Carlo method is used to verify the reasonableness of the results. Taking the prestressed concrete cable-stayed bridge as an example, the system degree is analyzed by DPIM-H as well as the reasonableness of the results is verified by Monte Carlo.

Multiphase flow and non-Newtonian fluid - Modelling and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PORE-SCALE STUDY OF MULTIPHASE FLOW PATTERNS IN LAYERED POROUS MEDIA WITH FRACTURES

Bo Li[*1], Hao Yu[1] and HengAn Wu[1]*

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ABSTRACT

The presence of fractures increases the difficulty of multiphase flow mechanism analysis, and it remains unclear how fractures affect multiphase flow displacement in the layered rock matrix. Herein, a pore-scale imbibition model considering the layered matrix-fracture system is established using the phase-field method, where oil is displaced by a range of fluids with various properties. Two typical flow modes are carefully analyzed, depending on the locations of the fracture and the interfaces between different layers of the matrix: fracture is parallel to the interface (mode I) and it penetrates through the interface (mode II), which are dominated by the co-current imbibition and counter-current imbibition mechanisms, respectively. Interestingly, the surface tension is found to be negatively correlated with the ultimate oil recovery rate for mode I and plays an opposite effect on that of mode II. For flow mode I, the conditions of lower injection rate, higher viscosity ratio, higher grain diameter ratio, and injection of the invading fluid from the larger pore throat size (positive direction flow) can improve oil recovery. For flow mode II, the fracture bifurcation angle has little effect on the positive direction flow, while it can significantly regulate the phase distribution in the negative direction flow. Based on the scaling analysis of relating pore-filling events to displacement modes and the equilibrium relationship between capillary and viscous forces, two theoretical models are derived to predict the imbibition patterns, and the variation of the flow regime under various parameters in the typical layered matrix-fracture models is systematically concluded.

IMAGE-BASED MESOSCOPIC SIMULATIONS OF ALLOYS

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ABSTRACT

Polycrystalline materials consist of aggregates of grains with varying lattice orientations and sizes separated by grain boundaries. The random morphological and crystallographic microstructure characteristics are responsible for the anisotropic behavior of polycrystalline microstructures and determine their macroscopic properties and performance. The mechanical properties of alloys, including stress and strain response and elastoplastic anisotropy, are significantly affected by morphological and crystallographic (grain orientation, etc.) features.

The present studies of the microstructure effect on mechanical properties and performance have certain limitations. Research methodologies are mainly limited to representative volume elements (RVEs)-based experimental observations. In practice, the microstructure characterizations exhibit a large degree of randomness during deformation processing, and microstructure randomness reveals polycrystalline materials' probabilistic properties and performance. Consequently, the vast size and number of the microstructure RVE necessary to build the process–structure–properties–performance (PSPP) linkages are computationally prohibitive and challenging to investigate. Meanwhile, the simplified polycrystalline microstructures, such as single crystals, bicrystals, Voronoi, and ellipsoid polycrystals, fail to capture all the statistical microstructure characterizations of the heterogeneous grains. Aa a result, the datasets between microstructural characteristics and mechanical properties and performance are unlikely to be built without sufficient data.

In this work, we propose a patch-based texture synthesis reconstruction algorithm to accurately capture the statistical microstructure characterizations of the heterogeneous grains. Then, the established computational plasticity FEM model combined with explicit characterization algorithms was used to perform quantitative analysis on Inconel 718 superalloy to fully understand the macroscopic properties and performance responses (ultimate tensile strength, Von Mises stress, ductile failure initialization and propagation) in terms of morphological, crystallographic, and boundary characteristics. Finally, the patch-based texture synthesis coupled with explicit characterization algorithms was developed to determine the ductile failure sets using the microstructural parameters, such as grain orientation and boundary characters.

Modeling friction and wear
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LOAD-AREA RELATION OF RANDOM ROUGH SURFACES FOR LARGE CONTACT FRACTION

Chengya Li[*1], Yue Ding[1], Xuan-ming Liang[1] and Gangfeng Wang[1]*

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ABSTRACT

Establishing the accurate load-area relation is pivotal for comprehending complex phenomena such as friction, wear, and thermal and electrical conduction, particularly for large contact fraction. Unfortunately, prevailing contact models often fall short in capturing behaviors across the entire contact regime due to the oversight of intricate asperity interactions, especially in high load level. In this investigation, we address the challenge by incorporating asperity interactions in both elastic and elastic-plastic contact. The actual random distribution of contacting spots with various sizes is simplified as a hexagonal distribution of identical spots sharing the same quantity and total area. Leveraging the perfect symmetry, a representative asperity is then simulated by finite element method and asperity interaction is incorporated through the periodic boundary condition. The load-area relation is calculated up to almost complete contact. It is interesting to find that surface morphology and material properties predominantly affect the initial linear relation at small contact fraction, and the interactions among asperities are closely related to contact fraction and lead to a larger load than that neglecting asperity interactions. By comparing with the theoretical prediction of an incremental equivalent contact model at initial contact, the load-area relation is extended for general rough surfaces. Direct simulations on typical rough surfaces verify the accuracy of the advanced load-area relation within a large range of contact fraction. This developed model provides an efficient method to predict the overall contact response of rough surfaces, significantly reducing the computational burden. The advancement serves as a robust foundation for in-depth analyses in tribology, laying the groundwork for a nuanced understanding of friction, wear, and sealing behaviors.

Boundary element methods: New theories and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BI-MATERIAL TOPOLOGY OPTIMIZATION FOR VIBRO-ACOUSTIC PROBLEMS BASED ON NON-NEGATIVE INTENSITY

Dan Li[*1] and Haibo Chen*[1]

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ABSTRACT

In this work, the non-negative intensity (NNI) method is applied to a large-scale vibro-acoustic interaction system using the fast multipole boundary element method (FMBEM), and a bi-material topology optimization method is constructed to minimize the integration of non-negative intensity on predefined surfaces. The NNI provides a field on the surface of the radiating structure, consisting of positive-only contributions to the radiated sound power, which avoids the near-field cancellation effects that otherwise occur with the sound intensity field [1]. To intuitively characterize the contribution degree of structural surface to far-field radiation and provide a theoretical basis for acoustic radiation analysis and design of large-scale vibro-acoustic interaction systems, the FMBEM is adapted to the NNI by calculating the eigenvalue solution of the symmetric acoustic impedance matrix using a two-stage solution method. The fast multipole algorithm is adapted to accelerate the calculation of matrix vector products of adjoint problems. The topology optimization of a large-scale submerged cylindrical shell model is realized using FMBEM [2]. The vibro-acoustic interaction system is first solved using a FEM–FMBEM model, and the resulting surface fields are then used in the FMBEM calculation of the NNI. The integration of the NNI on the predefined surface is selected as the objective function to design the radiation mode of the structural surface. A structural material interpolation model is established using the solid isotropic material with the penalization method, and the topological sensitivity formulation is derived based on the adjoint variable method. Numerical results confirm the effectiveness of the proposed optimization method in minimizing the integration of the non-negative intensity.

Keywords: FEM-FMBEM coupling analysis; topology optimization; non-negative intensity

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MULTI-PHYSICS FRACTURE ANALYSIS OF COMPOSITE LAMINATES BASED ON EXTENDED LAYERWISE METHOD

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ABSTRACT

An extended layerwise method (XLWM) is presented for the composite laminates with multiple delaminations and transverse cracks. The discontinuity of displacements and temperature induced by multiple delaminations is simulated by strong discontinuous function while the discontinuity of strain between dissimilar layers is modeled by a weak discontinuous function. Transverse cracks are modeled using classical Extended Finite Element Method (XFEM). And then, based on the XLWM, some mixed variational principle is employed or presented to derive the Euler equations and the discrete forms for the multi-physics fracture analysis of composite laminates. A fully coupled time integration method is developed based on the Newmark integration algorithm and Crank-Nicolson scheme, the multi-physics fields are solved simultaneously. The thermo-mechanical, thermo-chemo, thermo-chemo-mechanical, piezoelectric-mechanical, thermo-piezoelectric-mechanical and thermo-mechanical-curing-seepage coupling analysis are carried out numerically for the damaged composite laminates. Many numerical examples are studied to demonstrate the capabilities of static response, stress intensity factor and energy release rate for the composite plates, stiffened plates and sandwich plates.

Multi-scale, multi-rate damage and fracture: Models, experiments, and simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CREEP LIFE MODELLING OF NICKEL-BASED SINGLE CRYSTAL SUPERALLOY DD6 WITH MCRALY COATING

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ABSTRACT

Single-crystal superalloy is a crucial structural material widely employed in aerospace, energy, and petrochemical industries. High-temperature creep resistance is a critical indicator for evaluating alloys. In this study, a method for predicting the creep behavior of MCrAlY-coated DD6 single crystal alloy was proposed, and the influences of oxide layer thickness and inner wall temperature on the creep strain rate were investigated. The model was validated experimentally. The results indicate that the MCrAlY coating has a minimal impact on the high-temperature creep lifetime of [001]-oriented DD6 single-crystal superalloy. Pre-exposure treatment thickens the initial oxide layer of the coating, effectively extending the creep lifetime of the coated alloy, particularly at higher temperatures and stress levels. This underscores the effectiveness of pre-exposure treatment in increasing the creep lifetime of the MCrAlY-coated DD6 single-crystal superalloy system. The influence of inner wall temperature on creep lifetime follows a parabolic pattern. Excessively low inner wall temperatures reduce creep lifetime due to significant thermal mismatch stresses, while excessively high inner wall temperatures decrease creep lifetime because of changes in material properties at those temperatures.

Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TYPE Ⅰ TO TYPE Ⅱ TRANSITION IN SWEPT-FORWARD FIN SHOCK INTERACTIONS

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ABSTRACT

The transition from Type I to Type II in the swept-forward fin shock interaction is important, as it represents a shift from low to high heat flux interaction types. However, the mechanism for this transition remains unclear. In this study, theoretical and numerical analyses is employed to explore the transition mechanism. A theoretical model is developed to obtain the analytical solution for the transition condition, considering only the interaction of the incident shock and the bow shock of the fin on the symmetry plane. The theoretical solution is compared with numerical results at a freestream Mach number of 6.36. The results suggest that the transition occurs advanced, with three distinct transition mechanisms observed. At small wedge angles, the downstream flow pattern has an influence on the transition. In the downstream flow, the transmitted shock reflects on the wall as a Mach reflection. If the height of the Mach stem approaches the detachment distance of the fin shock, the transition occurs. At larger wedge angles, the transition occurs when the Mach number behind any one of the two transmitted shocks is less than 1. The other transition is observed at a wedge angle of 30°, which occurs accompanied by the disappearance of the supersonic jet.

Applications of shape optimization in complex engineering problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SHAPE OPTIMIZATION FOR LITHIUM-ION BATTERY WITH POROUS ELECTRODES

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ABSTRACT

In this presentation, we introduce a gradient-based shape optimization framework to design porous electrodes for maximum energy storage. Lithium-ion batteries are becoming increasingly important energy storage devices. Highly tortuous electrode materials can provide significant surface area per volume, which is required for large energy density. However, such a tortuosity can also deteriorate electrochemical transport, leading to poor material utilization in planar electrodes. Consequently, architecting electrodes that account for both transport and chemical activity is a promising alternative.

We consider a model with two materials: porous electrode and pure electrolyte. Density-based topology optimization has previously been used to design batteries for both half-cell and full-cell models to maximize energy storage. Despite the capability of producing complex interdigitated structures, an appropriate penalization scheme for intermediate materials is required for the optimizer to provide near binary designs. Setting up such a penalization is often time-consuming due to the large number of design-dependent variables that affect the forward model differently. Alternatively, the shape optimization approach used in this work produces binary designs naturally by morphing conformal meshes, circumventing inaccuracies associated with fuzzy interfaces. Shape sensitivities are computed via the adjoint method and leveraging automatic differentiation. The optimization problem is solved using a nonlinear programming technique.

In this presentation, we perform shape optimization on a half-cell model to maximize its energy storage when a fixed charging current is applied. We study multiple arrangements of physical parameters and compare their performance against a monolithic electrode. Both 2D and 3D results are presented.

Recent advances in computational fracture mechanics and failure analysis
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STUDY OF TIMOSHENKO BEAM-BASES CRANKSHAFT MODEL WITH NON-LINEAR BREATHING CRACKS

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ABSTRACT

With the development of the marine industry, marine diesel engines have the characteristics of complex structure and worse operating environment and frequently changing operating conditions, which put forward higher requirements on the index of shaft vibration. In the actual operation of a diesel engine, the crankshaft will generate three forms of vibration: bending, axial and torsion. These three forms of vibration are coupled with each other. Therefore, it is studied of the three-dimensional coupled vibration problems of the crankshaft system in this paper.

Firstly, the single crank is simplified as a five-segment straight beam structure. Based on the continuum vibration theory, the three-dimensional space field transfer matrix of the straight beam is derived. It is established for the point transfer matrices of coordinate transformation by using the conditions of displacement continuity and force equilibrium. The three-dimensional coupled vibration dynamic equation of the crankshaft system is constructed by using the multiplication of the transfer matrices. By taking modalities as generalized coordinates, there are simple representation for kinetic energy and potential energy of the vibration system. Lagrange equation is used to establish the differential equation of forced vibration of Simple crank system. The response of three-dimensional coupled forced vibration can be solved. A Timoshenko beam-based modelling method is proposed in this study, which considered the cross-section shape effect of the beam and non-linear breathing cracks are inserted as a spring potential energy term of the Lagrange equation.

Secondly, the finite element model of the crankshaft system was built by ANSYS WORKBENCH. The free vibration and forced vibration of the crankshaft system are calculated. The coupling vibration characteristics of the crankshaft system with non-linear breathing cracks under the burst force are analyzed. The results verified the correctness of the theoretical method in this paper.

Machine learning and data driven based engineering computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN MODELLING AND OPTIMIZATION METHOD FOR EFFICIENT MODELING OF COMPLEX STIFFENED CURVED SHELLS

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ABSTRACT

A data-driven modelling and optimization method is proposed to automatically model and optimize stiffeners on the complex stiffened curved shells. Firstly, a novel mesh-mapping method is developed for the data-driven modelling of complex stiffened curved shells based on radial basis function surrogate model. Secondly, an active learning-driven control point optimization method is proposed, which can improve the efficiency of modeling. Furthermore, a data-driven optimization approach, based on the deep neural network method, is employed to minimize the weight of the complex stiffened curved shells. Finally, two engineering examples are presented to verify the effectiveness of the proposed method, which reduces the modeling time by 84.9% and 66.3%, respectively, compared to using all control points in mesh-mapping. In conclusion, the proposed method has substantial potential in efficient modeling and improving engineering’s optimization efficiency.

Fracture, damage and failure mechanics of cementitious materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INVESTIGATION OF MESOSCALE FRACKING IN HETEROGENEOUS QUASI-BRITTLE MATERIALS USING A HYDROMECHANICAL COHESIVE PHASE-FIELD MODEL

Hui Li[*1] and Zhenjun Yang[1]*

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ABSTRACT

This study develops a mesoscale hydraulic fracturing modelling method combining a hydromechanical cohesive phase-field model with random field (RF) models and random aggregate models for simulating complicated 2D/3D mesoscale hydraulic damage and fracture in quasi-brittle materials. In this method, a Weibull RF generation algorithm is used to implicitly represent the material's fracture properties such as tensile strength and fracture energy, and its meso-structures such as aggregate, mortar, and interfaces are explicitly built using a random aggregate generating and packing algorithm and an aggregate scaling algorithm. The hydromechanical cohesive phase-field model is used to automatically model fluid-driven crack initiation and propagation in mesoscale models without remeshing. Monte Carlo simulations and parameter studies are then carried out to investigated the effects of mesoscale properties on fracking. A concrete cube under hydraulic pressures was analysed as an example. It is found that the predicted crack paths and fluid pressure curves both are stochastically affected by random fracture properties. A higher variance of tensile strength leads to a lower mean and larger standard deviation of peak pressures. Due to weaker fracture properties of aggregate-mortar interfaces than mortar, 3D hydrocrack tends to propagate along interfaces, leading to tortuous and non-planar crack paths after fracking.

CONFINEMENT EFFECTS ON THE THERMODYNAMICS AND FLUID FLOW IN POROUS MEDIA

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ABSTRACT

Unconventional shale recovery requires fundamental understandings of confinement effects on fluids flow behavior. Natural shales have complex pore network and chemical compositions, which prevent systematic study to understand the confinement effects. In this talk, we will present results from molecular simulations and provide insights into pressure-driven hydrocarbon fluid flow confined under amorphous silica pores. Coarse grained molecular simulations are performed to elucidate how confinements including the confinement size, shape, surface wettability, influence the thermodynamics and fluid transport in pores of single nanometer size. The force parameters of the adopted coarse grained molecular model are calibrated from the thermodynamic equation of state. Our numerical results demonstrated the importance of fluid-pore interaction, pore size, and pore morphology effects in mediating the pressure-volume-temperature (PVT) properties of hydrocarbons. Also, we found that the saturation pressure predicted from the van der Waals-type adsorption isothermal loop could be elevated or suppressed relative to the bulk phase. Based on the flow simulation results, a detailed analysis regarding the impact of each of these factors will be presented.

Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATION OF SOLID SHELL MATERIAL POINT METHOD IN EXTREME DEFORMATION OF THIN STRUCTURES

Jiasheng Li[*1] and Xiong Zhang*[1]

[1]*Tsinghua University*

ABSTRACT

Shell structures play a significant role in large-span situations. For safety and security, large deformation and destruction of shell structures has attracted great attention. With the large span of shell structures and inhomogeneous in material distribution, experiments of equal proportion are ordinarily expensive, while the corresponding results of the same experiment conditions may vary from each other. Therefore, the development of efficient and powerful algorithms to simulate complicated responses of shell structures remains an active field of research.

The standard material point method (MPM) has been applied to simulate shell structures. Several locking phenomena induced by the linear shape function will result in an overestimation of stress state and an underestimation of deformation when adopting a coarse background grid in the standard MPM. And thus, the discretization size of background grid should be small enough for shell simulations with the standard MPM, usually smaller than 1/5 of the shell thickness, which would lead to prohibitive computational cost.

A novel solid-shell material point method (SSMPM) is proposed in this work by introducing shell particles and locking treatments. The SSMPM adopts the shell particles to define the geometry of shell structures. A shell particle consists of a hexahedral particle domain, eight corners and Gauss quadrature points. Its deformation is obtained by solving the momentum equations on the background grid. For each shell particle, the assumed natural strain (ANS) method is adopted to eliminate shear locking and trapezoidal locking, and the enhanced assumed strain (EAS) method is employed to eliminate thickness locking. With the accurate description of bending modes, a single layer of shell particles and a coarse background grid are sufficient for shell structure simulations, which dramatically increase the computational efficiency. A local multi-mesh contact method is presented for contact situations. The advantages of MPM particles to simulate fragmentation and shell particles to simulate bending deformation are combined for extreme deformation of thin structures.

DEVELOPING AND ANALYZING A NOVEL UNCONDITIONALLY STABLE EXPLICIT FINITE ELEMENT METHOD FOR THE ELECTROMAGNETIC ROTATION CLOAK MODEL

Yunqing Huang[1], Jichun Li[2] and Bin He[3]*

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[2]University of Nevada Las Vegas
[3]Lanzhou Jiaotong University

ABSTRACT

One potential application of metamaterials is for designing invisibility cloaks. In this talk, I'll talk about a rotation cloak model. Here we carry out the mathematical analysis of this model for the first time. Through a careful analysis, we reformulate a new system of governing partial differential equations by reducing one unknown variable from the originally developed modeling equations in our previpous work [1]. Then a novel unconditionally stable explicit finite element scheme is proposed and its stability and optimal error estimate are proved. Numerical simulations are presented to demonstrate that the new scheme for the reduced modeling equations can effectively reproduce the rotation cloaking phenomenon. The talk is based on [2].

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Uncertainty quantification and reliability analysis in engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RESEARCH ON THE DYNAMIC RESPONSE OF OIL STORAGE TANK PLATFORM STRUCTURE UNDER THE EARTHQUAKE ACTION IN ICE REGIONS

Liang Li[*1]*

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ABSTRACT

In recent years, with the rapid development of China's economy, the importance of marine resources has become increasingly prominent. Oil storage tank platform structures play a fundamental role in the development of offshore oil and gas resources. These structures often face complex and harsh environments in ice-prone regions, including the threat of seismic excitation and seasonal sea ice. To ensure the safe operation of offshore platform structures, it is necessary to conduct research on the dynamic response of oil storage tank platforms in ice zones under seismic excitation. In addressing this issue, this study developed a non-freezing model ice that is representative of the Bohai Sea ice environment. Subsequently, underwater vibration table tests were conducted on the oil storage tank platform structure using the model ice in a model ice pool. A numerical model was also established to simulate the dynamic response of the oil storage tank platform structure under seismic excitation. The seismic response analysis of the oil storage tank platform structure in ice zones was conducted by combining the numerical model and experimental data.

Multiphysics biomechanics of bio- and bio-inspired soft materials: Theory, simulation and experiments
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SELECTIN AND INTEGRIN COOPERATIVELY REGULATE ROLLING ADHESION OF LEUKOCYTE UNDER SHEAR FLOW

Long Li[1] and Jizeng Wang*[1]

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ABSTRACT

Cell interacting with its extracellular matrix involves complex structures formation consisting of a multitude of proteins and often takes place in a hydrodynamic environment, e.g., leukocyte locomotion inside blood vessel in the process of inflammation. Despite the omnipresence of rolling adhesion of cell mediated by multiple type of proteins under hydrodynamic impact, the mechanisms underlying how the mechanics of multiple proteins cooperatively may govern the dynamics of cell rolling is not yet fully resolved. Here we present a mechanical model on rolling adhesion of cell mediated two distinct adhesive proteins in shear flow, corresponding to selectin- and integrin- jointly regulating leukocyte adhesion. Considering two pairs' binding/unbinding events as Markov processes and describing kinetics of leukocyte by the approach of continuum mechanics approach give rise to the mechanical description of rolling adhesion process. Through examining the dynamics of leukocyte rolling as a function of relative fraction of selectin and integrin pairs, we show that, during recruitment, the elongation of intermittent weak selectin bonds consuming the kinetic energy of rolling leukocyte decelerates the rolling speed and enables the integrin pairs to form strong bonds, therefore achieving the arrestment of leukocyte (firm adhesion). The coexistence of selectins and integrins may also be required for effective phase transition from firm adhesion to rolling adhesion, due to dynamic competition in pairs' formation and elongation.

Lattice Boltzmann modelling and study of complex flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL STUDY ON THE INNER WETTING MECHANISM FOR HYDROGEN-OIL SYSTEM IN THE POROUS MEDIA OF THE CATALYST PARTICLE WITH DIFFERENT SHAPE BASED ON THE PF-LBM

MengHui Li[12], Yumei Yong[2], Hanyang Mo[23], Wenqiang Chen[24], Jialin Dai[24] and Chao Yang[2]*

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[2]*Chinese Academy of Sciences*
[3]*China University of Mining and Technology-Beijing*
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ABSTRACT

The inner wetting characteristics in the catalyst particles have a significant impact on the activity and selectivity of catalysts[1]. Due to the complexity of the internal geometry structure of particles and the limitations of experimental conditions, the wetting condition inside particles remains unknown and assumed. Therefore, the paper numerically explored the wetting state and mechanism for hydrogen-oil flow in a catalyst particle by phase field lattice Boltzmann method (pf-LBM) developed by our team[2]. First, we randomly constructed irregular pore structures and reproduced the cross-sectional morphology of the catalyst particles. Combining the uniform distribution and Gaussian distribution, using the Voronoi edge topology to take the midpoint, doing spline interpolation to satisfy the random channel, and then verifying through tortuosity. There were 36 interpolation schemes dealing with the complex inner wall boundary condition. And the wettability condition was set at the inclinded planes which hydrogen, oil and inner wall contacted. After validating the pf-LBM, we simulated the oil wetting process in the porous media with different catalyst shape under different conditions. According to the numerical results, this work mainly focused on the effect of the catalyst geometry construct, fluid physical properties and operation conditions on the wetting area and efficiency. We studied the laws how the porosity, average pore diameter, tortuosity, catalyst shape, hydrogen/ oil physical properties, hydrogen/ oil ratio and driving force decided the oil distribution. A correlation about the inner wetting efficiency for the catalyst particles was presented. Thus the results are helpful to quantitatively master the inner wetting state and optimize catalyst geometry.

Key words: inner wetting efficiency; phase-field lattice Boltzmann method; geometric construct; porous media; two phase flow

Reference

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Applications of shape optimization in complex engineering problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

WRINKLED AND WRINKLE-FREE MEMBRANES

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ABSTRACT

Membranes are easy to buckle and wrinkle due to their extreme flexibilities, leading to the performance degradation and hampering the engineering applications. Here we propose a wrinkle-free approach through optimizing the shape and distribution of interior irregular holes in the membrane. A theoretical model with Marguerre function and complex analysis is performed to accurately estimate the stress distribution and wrinkling capability of the non-uniform membrane. The non-gradient particle swarm optimization (PSO) algorithm is implemented to determine the optimized holes to achieve wrinkle-free performance with ignorable area loss, the computational efficiency has been significantly enhanced through the superposition method. Both post-buckling analyses and physical experiments are carried out to verify wrinkle-free performance of membranes with optimized holes. In addition, an easy-to-implement empirical method is provided to guide the design of wrinkle-free membranes with arbitrary aspect ratio.

MULTI-PHYSICS HIGH-FIDELITY NUMERICAL SIMULATION METHODS FOR METAL ADDITIVE MANUFACTURING PROCESSES

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ABSTRACT

Metal additive manufacturing processes involve multi-physics interaction problems, including heat transfer, fluid dynamics, and solid mechanics. Such complexities challenge conventional numerical methods. This study introduces two novel numerical methods specifically designed to address the multi-physics problems in metal additive manufacturing processes. The first method, called the local multi-mesh finite volume method, efficiently handles heat transfer and melt pool dynamics. It utilizes a dual-mesh system to solve macroscopic temperature across the entire domain and mesoscopic heat and fluid dynamics within the melt pool vicinity. By employing a refinement-by-superposition paradigm, this method enables efficient simulations at the powder scale. The second method, known as the multi-physics material point method, effectively addresses thermo-fluid-solid interactions. It discretizes the material domain using a structured grid and a group of particles for heat transfer, fluid dynamics, and thermal stress solution under both Eulerian and Lagrangian frameworks. This method incorporates a semi-implicit local iteration for phase-changing heat transfer, a modified Chorin's projection method for Darcy's damping, and a staggered derivation scheme for Marangoni forces.

Numerical cases were conducted to validate these methods, and the results were compared with analytical, numerical, and experimental benchmarks. Notably, the local multi-mesh finite volume method demonstrated significantly improved computational efficiency, outperforming the traditional finite volume method by factors of 16 to 50. Furthermore, the multi-physics material point method achieved faster convergence in managing phase transitions, requiring 75% fewer iterations than the traditional bisection and Newton methods. The two methods present promising solutions for addressing the challenges of multi-physics phenomena in metal additive manufacturing.

Data-driven methods for modeling complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A PYTHON TOOLBOX FOR BAYESIAN LEARNING OF PORT-HAMILTONIAN SYSTEMS

Peilun Li[1], Kaiyuan Tan[1] and Thomas Beckers[1]*

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ABSTRACT

Machine learning has emerged as a powerful tool for modeling and control of dynamical systems across various scientific and engineering domains. Dynamical systems, characterized by their evolution over time, can exhibit intricate behaviors that are challenging to capture using first principal methods alone. Hence, utilizing data driven approaches to model complex dynamical systems can offer high accuracy and emerges as a generalizable method. However, for creating robust modeling and safe control of dynamical systems, machine learning approaches has often been hindered by their inherent limitation: a lack of consideration for the underlying physical laws and constraints that govern the behavior of any real-world dynamical system. As a result, the models often lack trustworthiness and generalizability.

In contrast, physics-informed machine learning leverages the inherent knowledge and understanding of the physical world to inform the learning process of machine learning algorithms. By explicitly integrating physical laws, domain expertise, and prior knowledge into the learning framework, physics-informed learning empowers control systems to leverage the flexibility and adaptability of machine learning while remaining grounded in a solid understanding of the underlying dynamics.

In the talk, we will introduce PyGpPhs – an easy-to-use toolbox for physics-informed learning of electromechanical systems. The toolbox is built on our recently introduced Gaussian Process Port-Hamiltonian systems (GP-PHS) which is a physics-constrained, nonparametric Bayesian learning approach with uncertainty quantification. In contrast to many other physics-informed techniques that impose physics by penalty, the proposed data-driven model is physically correct by design. The Bayesian nature of GP-PHS uses collected data to form a distribution over all possible Port-Hamiltonian systems instead of a single point estimate. Thus, the GP-PHS model i) generalizes well, ii) is highly interpretable and iii) the inherent uncertainty quantification enables future safe model-based control approaches. To further demonstrate theory and usages of the toolbox, we will present the learning of the dynamics of a non-harmonic oscillator in detail. The toolbox is easy to use and demonstrate high accuracy in modeling.

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Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHASE FIELD FRACTURE MODEL AND TOPOLOGY OPTIMIZATION FOR ADDITIVE MANUFACTURING

Qing Li[1], Chi Wu[1], Cuiyi Li[2], Jianguang Fang[2] and Grant Steven[1]*

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ABSTRACT

Phase field models have been extensively studied in the analysis of brittle and ductile fracture. However, few have been explored to simulate additively manufactured materials and validated by experimental data so far. This study develops a phase field framework for modelling complex mechanical behaviours of 3D printed metallic and ceramic materials [1]. To consider the 3D printing induced microstructural orientation, transversely isotropic Hill48 and modified Mohr-Coulomb constitutive models are incorporated here to depict the plastic and fracture behaviours, respectively. The numerical results divulge that, by considering the stress state-dependent crack initiation, the proposed phase field model can better simulate the force-displacement responses [1]. Remarkably, the complex fracture sequences, including crack initiation, propagation, and final rupture, can be properly simulated by the proposed phase field model. Importantly, it is necessary to apply a transversely isotropic fracture model to characterise the orientation-dependent fracture behaviour.
Further, the phase-field damage model established is incorporated into the topology optimization framework to consider crack initiation and propagation in a path-dependent fashion [2,3]. The topological design enables to enhance fracture resistance of structures made of additive manufacturing components. A path-dependent shape derivative is developed in a step-wise manner during the nonlinear fracture analysis, which enables to drive the topology optimization properly [3]. To measure the fracture resistance of structure, a p-norm function is formulated to aggregate the phase-field variables into a single constraint. The numerical examples demonstrated that the proposed phase field based topology optimization method can significantly improve the fracture resistance of additively manufactured structures [2]. The proposed method is anticipated to provide an effective approach for sophisticated path-dependent topological design of structures reducing severe stress concentration and high risks of fracture failure.

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Computational mechanics in Canada and China: Current states of shared scientific interests and opportunities for the future cooperation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RECENT PROGRESS IN REACTIVE DIFFUSION MODELLING FOR FLEXIBLE BIOELECTRONIC SYSTEMS

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ABSTRACT

Flexible bioelectronics is a class of technology that involves components which physically disappear, in whole or in part, at prescribed rates and at programmed times. Enabled devices include medical monitors that fully resorb when implanted into the human body (“bio-resorbable”) to avoid long-term adverse effects, or environmental monitors that dissolve when exposed to water (“eco-resorbable”) to eliminate the need for collection and recovery. Theoretical modeling of the behaviors of the constituent materials represents important design tools for flexible bioelectronic systems. In this talk, a class of reactive diffusion models for the analyses and designs of flexible bioelectronic systems are reported, by which the key quantities such as the distribution of water concentration, thickness change, and lifetime predictions are obtained analytically. These models are well validated by the experiments and provide effective approaches to innovative designs of related devices.

Machine learning and multiscale modeling for complex materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT OF VARIATIONAL BAYESIAN LEARNING NEURAL NETWORK FOR SOLUTIONS OF INVERSE PROBLEMS: FROM FORENSIC ANALYSIS OF TRAFFIC ACCIDENTS TO THERMAL DISTORTION CONTROL IN 3D PRINTING

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ABSTRACT

We have developed a class of variational Bayesian learning neural networks-based machine learning algorithms, including a mixed Bayesian variational finite element method, to solve various inverse problems, such as reconstruction of car crash accidents, thermal distortion control in 3D printing, and general structural forensic analysis on fracture and crack propagation. In this work, powerful variational Bayesian learning-based computation algorithms have been developed to “inversely” identify the deformation maps in the sense of continuum mechanics as well as the loading conditions while the only information given is the deformed material shape or geometry.

We developed several novel techniques, such as (1) Variational Bayesian Learning formulation coupled with a Feed-forward architecture, and (2) a mixed Galerkin variational Bayesian learning finite element method and its inverse solution for deformation mappings in any dimension. We have then applied these computational algorithms to several important real engineering applications. We have demonstrated that the developed machine-learning algorithm can practically identify the deformation field of a real crashed car and recover its initial pre-crash state based on residual damaged geometric configuration, and the Bayesian regularization network can provide a powerful geometric deviation control (BRN-GDC) algorithm that has the capability to control the thermal distortion in 3D printing that is parameter- and location-dependent.

In this talk, we present an overview of the theory and computational algorithms of Variational Bayesian learning neural network methods and their applications.

Advanced numerical methods for the modeling and optimization of coupled dynamical systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THERMOELASTIC DAMPING OF FGM MICRO BEAMS BASED ON THE HIGHER-ORDER SHEAR DEFORMATION THEORY

Shirong Li[1] and Zeqing Wan*[1]

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ABSTRACT

Thermoelastic damping (TED) in free vibration of a simply supported functionally graded material (FGM) micro beam with rectangular cross section is investigated based on the classical thermoelasticity. Material properties of the FGM micro beam are assumed to be continuously vary along the beam thickness. Governing equations for the structural vibration coupled with the temperature field are formulated by using Levinson higher-order shear deformation beam theory. Heat conduction equation coupled with the bulk strain is derived on the basis of Fourier model. For small amplitude transverse vibration, we assume that heat conduction effect is dominant in the thickness direction so that the heat conduction equation is simplified as a quasi-one-dimensional differential equation with variable coefficients which are functions of the coordinate in the beam thickness direction due to the transverse inhomogeneity of the materials. A layer-wise homogenization approach is employed to approximately solve the heat conduction equation with variable coefficients, where the FGM beam is divided into numerous uniform layers where the thermal and mechanical properties in each layer are considered to be constant and evaluated at the mid-surface of the divided layer. Consequently, the heat conduction equation possessing variable coefficients is discretized into a series of differential equations with constant coefficients in each layer. Analytical solutions for these equations with the adiabat boundary conditions at the beam top and bottom surfaces and the continuation conditions at the interfaces are obtained in terms of the kinematic quantities. Afterwards, the TED in the FGM Levinson beam is determined by the complex frequency approach in terms of the isothermal frequency of the homogenous Euler-Bernoulli beam by using mathematical similarity between the eigenvalue problems for the two types of beams. Considering an FGM beam with the material properties varying as power functions from full silver (Ag) at the top surface to full silicon (Si) at the bottom one, numerical results are presented to quantitively analyze the effects of the material gradient, the geometry and the shear deformation on the TED and the frequency shift of the micro beams in detail. The numerical results show that the TED evaluated by the Levinson beam theory (LBT) is smaller than that by the Euler-Bernoulli beam theory (EBBT) and the difference becomes significant along with the increase in the value of the thickness-to-length ratio. Therefore, for a thick or moderately thick micro beam the LBT can provide a more accurate prediction for the TED than the EBBT.

Numerical modeling of granular and multiphase flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A DATA-DRIVEN MULTISCALE SURROGATE MODEL FOR CFD–DEM SIMULATIONS

Shuo Li[1] and Mikio Sakai*[1]

[1]*The University of Tokyo*

ABSTRACT

Gas–solid flows are commonly investigated in industries. The CFD–DEM method is an established method for simulating the gas–solid interactions. However, the CFD–DEM simulation of industrial gas–solid flows often requires substantial computational resources. To address this issue, in this study, a novel data-driven multiscale surrogate model, referred to as a reduced-order model coupled with a signed distance function-based graph network (ROM–SGN), is proposed to accelerate the simulation of gas-solid flows. Validation studies are conducted in a fluidized bed. Macroscopic properties such as particle distribution, pressure drop, and bubble distribution are compared between the CFD–DEM and ROM–SGN simulations. The results demonstrate that the ROM–SGN accurately simulates the gas–solid dynamics and significantly reduces calculation time by several orders of magnitude compared to CFD–DEM simulation. This work will contribute significantly to the advancement of simulation and modeling for industrial multiphase flows.

Keywords: CFD–DEM; Surrogate model; ROM–SGN; data-driven coupling.

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Recent advances on interfaces dynamics modeling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A SIMPLE MODEL FOR SIMULATING VESICLE EXPANDING AND SHRINKAGE

Shuwang Li[*1], Steve Wise[2] and Xiaoxia Tang[1]*

[1]*Illinois Institute of Technology*
[2]*University of Tennessee*

ABSTRACT

In this talk, we present a diffuse interface model for vesicle expanding (growth) or shrinkage induced by an osmotic pressure. The model consists of an Allen-Cahn equation describing the evolution of the phase field and a Cahn-Hilliard equation describing the evolution of the concentration field. We establish control conditions for expanding or shrinking vesicles using the concept of common tangent construction in materials science, allowing the exchange of materials between the interior and exterior domains. Numerical experiments reveal that the model can capture the main feature of dynamics: formation of circle-like (expanding) and finger-like (shrinking) vesicles.

Microstructures of chemically complex materials and their impacts on material properties from multiscale simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CURVATURE-CONTROLLED BAND ALIGNMENT TRANSITION IN 1D VAN DER WAALS HETEROSTRUCTURES

*Wenbin Li**[1]

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ABSTRACT

One-dimensional (1D) van der Waals (vdW) heterostructures of coaxial inorganic nanotubes, such as carbon nanotubes and transition metal dichalcogenide (TMDC) nanotubes, have recently emerged as a new area of endeavor in materials science. A key prerequisite for designing the properties of 1D vdW heterostructures is to understand the band alignment of the coaxial nanotubes in these novel heterostructures. In this talk, I will present our recent first-principles study of the effect of curvature on the electronic structure and band alignment in 1D vdW heterostructures of TMDC nanotubes. We find that, as the diameter of an individual TMDC nanotube decreases, the combined effect of curvature-induced flexoelectricity and circumferential tensile strain causes a rapid lowering of its conduction band minimum, while the valence band maximum exhibits an initial lowering before rising. As individual TMDC nanotubes form coaxial heterostructures, the concerted effect of diameter-dependent band-edge levels and intertube coupling via flexovoltage can lead to a Type II to Type I transition in intertube band alignment in several 1D TMDC heterostructure systems, including large-diameter MoSe2@WS2, MoTe2@MoSe2, and MoTe2@WS2 heterostructures. The results lay down a foundation for the rational design of 1D vdW heterostructures.

Machine learning and data driven based engineering computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BIOMIMETIC CELLULAR MATERIAL UNIT CELL REPRESENTATION AND ON-DEMAND DESIGN BASED ON A TRANSPARENT NEURAL NETWORK AND A NEURAL OPERATOR

Xiang Li[1], Ziming Yan[2], Zhanli Liu[2] and Zhuo Zhuang[2]*

[1]*Hainan Normal University*
[2]*Tsinghua University*

ABSTRACT

Cancellous bone is a natural cellular material that is able to proactively change its microstructure to adapt to the surrounding loading conditions. This adaptability gives the bone anisotropic mechanical properties and the ability to absorb energy. Inspired by the topological and mechanical properties of cancellous bone, this research proposes a framework to represent and design biomimetic cellular materials based on a transparent neural network and a neural operator. In this research, a transparent neural network is used to compute the Gaussian random field and generate the topology of the spinodoid, a biomimetic cellular material. Furthermore, a novel homogenization method accelerated by neural operators is presented to efficiently compute the anisotropic elastic matrices of the spinodoid unit cells, combining improved computational speed with precision. Finally, a data-driven workflow is introduced to inversely determine the topological parameters of the spinodoid unit cell based on the given anisotropic elastic matrix. Numerical examples show that the proposed framework is capable of efficiently and correctly designing spinodoid unit cells with given design goals and can be extended to the design applications of other biomimetic cellular materials.

Recent advances on interfaces dynamics modeling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FRONT TRACKING AND APPLICATION TO PARTACHUTE SIMULATION

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ABSTRACT

We introduce an integrated computational method for the simulation of the parachute system using the front tracking methodology. A dual-stress spring-mass model based on the front tracking method is used to study the dynamics of fabric surfaces in air. The numerical algorithms for this complex physics system includes fabric model and its coupling with the fluid solvers, both incompressible and compressible. The fabric porosity is modeled by the ghost cell method. The collisions, including fabric-fabric, fabric-rigid, rigid-rigid and string collisions with fabric and rigid are implemented. This presentation will introduce on the algorithms and simulation of the
supersonic parachute simulation. We will also present other applications, including fluid interface instabilities, phase transition and particle tracking with the front tracking software library.

Modeling and simulation of dynamics, stability and control of aerospace structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ANALYSIS ON NONLINEAR WHEEL-HOLDING CONTACT ON NOSE LANDING GEAR DYNAMICS CHARACTERISTICS DURING NEW TOWING-OUT MODE OF AIRCRAFT

Xiaoyun Li[*1], Yijun Chai[1], Xiongwei Yang[1] and Yueming Li[1]*

[1]Xi'an Jiaotong University

ABSTRACT

The safety and efficiency of airports are compromised due to civil aircraft commonly using their own engines for taxiing in the current era. A new generation of towing-out mode has been introduced, which utilizes the external power supplied by a towbarless tractor. A complex constraint relationship exists between the nose landing gear's wheel and the wheel-holding mechanism of the tractor during this towing process. The nose landing gear, a crucial component for ground taxiing, possesses dynamic characteristics that directly influence the safety of high-speed taxiing and the service life of the structure. Given the constraint relationship of wheel-holding contact force, it is imperative that a study be conducted on the vibration characteristics of the nose landing gear, which is subjected to both heavy load and towing load. A specific type of civil aircraft front landing gear is selected as the research subject, and a mathematical model is derived to describe the constrain between the nose landing gear's wheel and the wheel-holding mechanism. This derivation is based on the wheel-holding contact geometric relationship and the Winkler contact model. The static and dynamic characteristics of the nose landing gear under heavy load are investigated. Considerations are given to the wheel-holding contact interaction during towbarless towing, the nonlinear axial force of the shock absorber, and the buffering effect of the tractor tire. The influence of wheel-holding contact stiffness and nonlinearity on the vibration characteristics of the structure is also examined. A nonlinear relationship between the radial force and radial deformation of the wheel is revealed by the results, with the degree of nonlinearity inversely proportional to the radius of the clamping rod. As the wheel-holding contact stiffness increases, frequency veering and mode conversion are gradually experienced by the first and second modes of the nose landing gear under full-load towing conditions. The occurrence of frequency steering is observed when a specific nonlinear function relationship is exhibited between the clamping contact force and the stiffness of the tractor tire. Moreover, the nonlinearity of wheel-holding contact stiffness exerts a more pronounced impact on the first-order natural frequency of nose landing gear. The findings of this study can serve as a valuable reference for optimizing the nose landing gear under the new towing-out mode and designing the wheel-holding mechanism.

Numerical methods, mathematical modeling and analysis in material science
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INFER EXPLICIT NUMERICAL SCHEMES FROM IMPLICIT DATA WITH APPLICATIONS TO DEFECT DYNAMICS

Xingjie Li[*1], Fei Lu[2], Molei Tao[3] and Xiaofeng Felix Ye[4]*

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ABSTRACT

Efficient simulation of SDEs is essential in many applications, particularly for ergodic systems that demand efficient simulation of both short-time dynamics and large-time statistics. However, locally Lipschitz SDEs often require special treatments such as implicit schemes with small time-steps to accurately simulate the ergodic measure. We introduce a framework to construct inference-based schemes adaptive to large time-steps (ISALT) from data, achieving a reduction in time by several orders of magnitudes. The key is the statistical learning of an approximation to the infinite-dimensional discrete-time flow map.

We use the classical numerical schemes to derive informed basis functions, leading to a parameter inference problem. We introduce a scalable algorithm to estimate the parameters by least squares, and we prove the convergence of the estimators as data size increases. The numerical tests confirm that ISALT can tolerate time-step magnitudes larger than plain numerical schemes.

Recent advances in computational fracture mechanics and failure analysis
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL SIMULATION METHOD FOR FATIGUE CRACK PROPAGATION IN CLADDED C(T) TEST SPECIMEN

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ABSTRACT

To improve the corrosion resistance and rust prevention properties of nuclear reactor pressure vessel (RPV) in nuclear power plants, stainless steel is welded on the inner surface of vessel as cladding. In such cladded structure, due to the dissimilar material interface, fatigue crack propagation behavior is complex and further researches are required.

In this study, a numerical simulation method based on extended finite element method (XFEM) for fatigue crack propagation in cladded structure is proposed. This method employs 8-node hexahedral continuum elements enriched with only Heaviside step function, which can model planar crack independently of finite elements. For the crack across dissimilar material interface in cladded structure, first, the stress intensity factors along the crack front are evaluated by domain integral method, and then crack front shapes are updated by using Paris' law and then smoothed by the cubic Bezier curves in each region. The crack propagation analysis is performed by repeating this series of processes mentioned above.

In this presentation, fatigue crack propagation analyses for cladded C(T) test specimens are performed. The obtained relationships between crack length and load cycle as well as transition of propagating crack front shapes are compared with those of experiment and validated. It was shown that the proposed method appropriately simulated the fatigue crack growth behaviours in cladded C(T) test specimens.

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NUMERICAL SIMULATION OF THE COMPRESSIBLE STABLE RAYLEIGH-TAYLOR-KELVIN-HELMHOLTZ INSTABILITY WITH DISCRETE BOLTZMANN METHOD

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ABSTRACT

The Rayleigh-Taylor (RT) and Kelvin-Helmholtz (KH) instabilities are typical fluid instability phenomena that often occur in conjunction. The coupled RTKH system can be categorized as stable or unstable, depending on whether the heavier fluid lies beneath or above the lighter one. In stable RTKH systems, the evolution of physical fields is often accompanied by complex phenomena such as nonlinearity, multiscale effects, and nonequilibrium behavior. These complexities pose challenges for traditional methods. As a mesoscopic method, the discrete Boltzmann method (DBM) is capable of describing both hydrodynamic and thermodynamic behaviors and has recently been applied to study the RTKH instability[1-2]. In this study, we utilize the DBM to investigate the competition mechanism between the suppression and promotion of interface evolution, where stable RT inhibits interface evolution, while KH promotes it. This work aims to enhance our understanding of the nonequilibrium evolution of compressible stable RTKH instability and contribute to the theoretical framework of fluid instability.

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Mechanobiology of cells, vesicles and biomembranes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ANALYZING THE LONG TERM BIOMECHANICAL RESPONSE OF ORTHOKERATOLOGY BY CONSIDERING THE ANISOTROPIC VISCOELASTIC BEHAVIOR OF THE CORNEA

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ABSTRACT

Orthokeratology, an effective myopia correction and control technique widely adopted among adolescents, is increasingly gaining scientific attention. Most existing research focused on analyzing patient corneal morphology data to discern deformation patterns but often fell short in understanding the underlying biomechanical mechanisms. This limitation resulted in the fitting of orthokeratology lenses heavily relying on clinicians' judgment, posing a significant challenge for accurately predicting orthokeratology outcomes, i.e., corneal deformation. This study aims to reveal the mechanisms of orthokeratology by establishing a biomechanical model, facilitating the prediction of corneal deformation. We began by collecting extensive corneal morphological data from clinical myopia patients, based on which we constructed a geometrically personalized finite element model. This model considers the anisotropic, visco-hyperelastic mechanical properties of the cornea. It was validated by simulating the long-term response in central corneal thickness over an 8-day orthokeratology period and comparing these results with experimental data. Furthermore, the study explored the effects of corneal anisotropic characteristics and posterior surface boundary conditions on the shaping process. Corneal shear dominated by indentation was revealed as the key deformation mechanism in orthokeratology. Using this model, we analyzed the effects of lens-wearing time and cycle duration of orthokeratology lenses on myopia correction and proposed appropriate lens-wearing strategies for various degrees of myopia. The biomechanical model established in this research successfully captured the long-term viscoelastic response of central corneal thickness, laying a solid foundation for the quantitative prediction of orthokeratology outcomes.

Machine learning and multiscale modeling for complex materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HIGH-THROUGHPUT SCREENING AND PREDICTION OF HIGH MODULUS OF RESILIENCE POLYMERS USING EXPLAINABLE MACHINE LEARNING

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ABSTRACT

The ability to store and release elastic strain energy, as well as mechanical strength, are crucial factors in both natural and man-made mechanical systems. The modulus of resilience (R) indicates a material's capacity to absorb and release elastic strain energy, with the yield strength (σy) and Young's modulus (E) as R = σy2/(2E) for linear elastic solids. To improve the R in linear elastic solids, a high σy and low E combination in materials is sought after. However, achieving this combination is a significant challenge as both properties typically increase together. To address this challenge, we propose a computational method to quickly identify polymers with a high modulus of resilience using machine learning (ML) and validate the predictions through high-fidelity molecular dynamics (MD) simulations. Our approach commences by training single-task ML models, multitask ML models, and Evidential Deep Learning models to forecast the mechanical properties of polymers based on experimentally reported values. Utilizing explainable ML models, we were able to determine the critical substructures that significantly impact the mechanical properties of polymers, such as E and σy. This information can be utilized to create and develop new polymers with improved mechanical characteristics. Our single-task and multitask ML models can predict the properties of 12 854 real polymers and 8 million hypothetical polyimides and uncover 10 new real polymers and 10 hypothetical polyimides with exceptional modulus of resilience. The improved modulus of resilience of these novel polymers was validated through MD simulations. Our method efficiently speeds up the discovery of high-performing polymers using ML predictions and MD validation and can be applied to other polymer material discovery challenges, such as polymer membranes, dielectric polymers, and more.

CHARACTERIZING CYCLIC INELASTIC BEHAVIOR OF ANGLE MEMBERS: A MODIFIED HYSTERETIC MODEL

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ABSTRACT

Predicated on the Dicleli physical model [1], a modified hysteretic model tailored for displacement-controlled cyclic loading is devised. Comparative analysis through a finite element model indicates that the interrelation between normalized axial and lateral displacements solely depends on slenderness, ensuring the physical interpretation of the equation's parameters. Additionally, the study also explores the way local buckling alters cross-section shape and macroscopic component behavior. The new model reduces this impact with effective width. Given that the residual lateral displacement of each loading cycle may transform a straight rod into a bow-shaped rod, aggravating second-order effects and triggering early buckling. The improved model integrates geometric nonlinearity by updating the tangent modulus after each cycle, except initial imperfection, which is already included in the derivation of physical model. Since subsequent simulations demonstrate that low cycle fatigue damage and fracture propagation minimally affect the component's hysteresis curve, these factors are excluded from the model. The modified hysteretic model, validated by experimental tests and finite element simulations, effectively captures the key numerical values of the hysteresis curve, enabling a smooth transition from regular to random loading. This study offers a promising methodology for representing the cyclic inelastic behavior of angle members in various structures.

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Multiphysics and data-driven modeling for cardiovascular biomedicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AI-ENABLED RAPID IMAGE-BASED HEMODYNAMIC MODELING AND SIMULATION

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ABSTRACT

Cardiovascular disease (CVD) has persisted as a leading global cause of mortality for decades. While image-assisted computational fluid dynamics (CFD) simulation has proven invaluable in offering comprehensive hemodynamic insights for non-invasive diagnosis and clinical treatment planning for CVD, the conventional approach faces significant challenges hindering its widespread application. Firstly, the manual extraction of geometries from medical images is time-consuming, inconsistent among different operators, and may introduce human artifacts during geometry reconstruction. Secondly, the meshing, case setup, and execution of CFD simulation under realistic settings (e.g., high spatial and temporal resolution, fluid-solid interaction (FSI), Wind-Kessel boundary conditions) can be time-demanding, limiting its applicability in clinical scenarios requiring timely feedback or iterative model queries for device implant design. Thirdly, uncertainties in boundary conditions or model parameters during CFD simulation can compromise result credibility, reducing its effectiveness in clinical diagnosis.

In response to these challenges, we introduce a novel AI-enabled image-based computational modeling framework for automatic patient-specific image segmentation and rapid hemodynamic simulations, which harnesses the potency of deep learning to enable fast prediction of 3D blood flow patterns from raw image scans. Firstly, we automate vessel segmentation in medical imaging by developing a Laplacian-of-Gaussian (LoG) based Bayesian network, enhancing segmentation accuracy across diverse vascular structures. Subsequently, a shape deformation model using graph neural network (GNN) with residual connection reconstructs high-quality patient-specific simulation-ready meshes from segmented voxel images. Surface smoothness on the reconstructed geometry is ensured through the use of a large deformation diffeomorphic metric mapping (LDDMM) method. Finally, a GNN-based CFD surrogate model is established for rapid prediction of simulation results, handling unstructured meshes and featuring full gradient tracking and backpropagation for swift model adjustments and parameter optimization across complex vascular structures. The proposed models are demonstrated on a main aorta with upper branches (brachiocephalic trunk, left common carotid artery, and left subclavian artery), showcasing its merit and effectiveness. This study serves as a compelling indication that the integrated machine learning technologies hold substantial promise and have the potential to revolutionize CVD diagnosis, offering a more effective and efficient tools for cardiovascular healthcare.

Machine learning and multiscale modeling for complex materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTIPHYSICS-INFORMED MACHINE LEARNING FOR ARCHITECTED BATTERY DESIGN

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ABSTRACT

Li-ion batteries (LIBs) are critical for electrification in a wide range of applications to reach zero-net emission goal. These increasingly widespread applications warrant an improvement in the existing battery designs so as to meet this increasing demand. One such possible improvement is the use of Si anode instead of the traditionally used graphite electrode as this change allows for increased battery life, increased capacity, increased safety and better performance. The unique intercalation mechanism of Li ions into the Si anode Si anode results in a better specific capacity of the battery. In this mechanism Si atoms react with lithium, which leads to the bonds between the Si atoms giving way for the formation of the LixSi alloy. However, there is a cost associated with this design improvement. Volumetric changes of upto 300% are observed in the Si anode during the lithiation/delithiation cycles which results in the development of large internal stresses in the anode. Delamination of the Si anode from the current collector substrate and the cracking in the Si anode material itself are the consequences of this volumetric stresses, which causes a reduction in the capacity of the battery. The growth of the solid electrolyte interface (SEI) layer is another capacity fade mechanism that is coupled with mechanically induced damage in the LIBs. SEI layer growth in LIBs can lead to the increase in the internal resistance of the cell and the removal of the active Li material from the cycling process. The growth of the SEI layer on the surface of the anode mainly occur during the battery cycling phase. The continued growth of this layer increases the overall resistance and removes the active Li from the cycling system, thereby reducing the overall capacity of the battery. Hence, to be able to truly utilize Si as the active material for the LIBs, there is a tremendous need to understand these three coupled failure modes in the battery and identify electrode design that can mitigate the mechanically induced capacity degradation. One potential solution is architected electrode. In this study, multiphysics-informed machine learning has been developed to investigate the capacity degradation of architected electrodes with various designs under different operating conditions. This is the first work that can consider all major coupled failure models of Si-based electrodes in the performance analysis, which can facilitate the design of high efficiency battery with architected electrodes.

Fracture, damage and failure mechanics of cementitious materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SYNERGISTIC EFFECTS OF ENVIRONMENTAL DETERIORATION ON FATIGUE AND FLEXURE PROPERTIES OF GLASS FIBER REINFORCED POLYMERIC (GFRP) COMPOSITES : A MULTISCALE AND MULTIPHYSICS MODEL.

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ABSTRACT

This study aims to simulate synergistic UV & moisture deterioration and demonstrate its role in changing the residual fatigue and flexure performance in architectural GFRP composites. This study develops an experimentally validated 3D Multiphysics model at structural level and gets this homogenization-based model to identify each of the degradation mechanisms observed in the experimental data and to analyze the differences that the various degradation mechanisms might make to the properties and durability of the environmental aged composite materials. Sensitivity analyses are conducted to investigate the effect of mesh density on the accuracy of functions homogenized from micromechanical models. The aging-fatigue-bend model with respect to two different deterioration mechanism assumptions is developed and analyzed. Research shows that models with homogeneous damage assumptions allow higher feasibility and convergence when aging concurrently with complicated mechanical loading, while models with surface erosion assumptions describe the actual deterioration mechanism more precisely and offer more freedom, especially when the environmental aging condition is more complicated.

This model can be incorporated into many commercial finite element codes for a sustainability study of composite structures/systems. In future work, the models developed in this study will be combined with life cycle assessment (LCA) tools to support better sustainability-focused new material design, thus reducing costs and environmental impacts in the built environment.

NUMERICAL SIMULATION METHODS AND DATA-DRIVEN MODELS FOR METAL ADDITIVE MANUFACTURING

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ABSTRACT

Metal additive manufacturing (AM) technologies have found the potential to revolutionize the global part manufacturing landscape for their tremendous advantages in building geometrically complex parts with tailorable microstructures and properties. However, they still suffer from unexpected formation defects of the as-built geometry, dimension, and material properties, which require a complete understanding of the process-structure-property relationship. Because the process of metal AM involves extremely multi-physical phenomena taking place at a variety of temporal and spatial scales, high-fidelity numerical simulations are preferred to the costly trial-and-error experiments to address the process-microstructure-property relationship of AM and to aid the process parameters optimization for reducing the final product defects such as surface roughness, void formation, heterogeneous grain structures, etc. In this study, we proposed multi-scale and multi-physics numerical simulation methods, including the proposed multi-physics material point method, extended cellular automaton method, crystal plasticity finite cell self-clustering analysis method, for the powder melting-solidification process, grain structure evolution, and mechanical properties for different as-built alloys with different metal AM processes. The predictions from the proposed computational methods are in good agreement with the experimental data available in the literature for both powder bed fusion and wire-based directed energy deposition processes. Furthermore, data-driven models based on deep learning algorithms for the process-structure-property problems are developed based on the dataset by the proposed numerical simulation methods. The high efficiency and accuracy of these models are demonstrated. It is shown that the proposed methods and models can shed light on the process-microstructure-property relationships and can be further applied to optimizing process parameters.

Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A UNIFIED THEORY FOR SHEAR DEFORMABLE COMPOSITE PLATES

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ABSTRACT

A shear deformation-based unified theory for composite plates is established. The theory contains four unknowns which are explicit to interpret the physical response. Apart from the three common displacement components for a point on the midplane, a remaining higher-order displacement component is exclusively attributed to transverse bending and shear deformation. The transverse shear deformation of the function distribution can be represented by general shape functions. The elucidation of the thickness locking mechanism relies on the innovative displacement component introduced in this study, which improves the kinematic assumptions inherent in conventional plate/shell theories. Further, the present theory explicates the explicit physical terms associated with transverse normal stress and strain. In addition, the present unified theoretical framework, along with the corresponding assumptions, induces further simplification and transition into the conventional plate theories, namely, first-order shear deformation theory (FSDT), higher-order shear deformation theory (HSDT), and others. Exact analytical solutions of composite plates are obtained. A comprehensive numerical investigation has been performed, encompassing diverse plate theories and various composite structures, including functionally graded material (FGM) plate structures, FGM sandwich plate structures, etc. The clarity and unity in the present theory and the physical meanings can be elaborated by integrating the conventional theories under certain assumptions.

Recent advances in high-order methods for computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SPECTRAL DIFFERENCE SOLUTIONS OF TWO THREE-DIMENSIONAL KINEMATIC DYNAMO PROBLEMS

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ABSTRACT

We report a recent development of the high-order spectral difference method with divergence cleaning (SDDC) for accurate simulations of two 3D kinematic dynamo benchmark problems on unstructured grids consisting of high-order iso-parametric hexahedral elements. The divergence cleaning approach is based on the improved generalized Lagrange multiplier (GLM), which is thermodynamically consistent and Galilean invariant. The Spectral Difference with Divergence Cleaning (SDDC) method has been used to successfully model a number of nonlinear MHD problems. The spectral difference method is a versatile high order method that can be used for unstructured grids and can be massively parallelized. The first kinematic dynamo problem was solved in a cubic box with all periodic boundary conditions. The SDDC method will be verified to capture the “Cigar” structures published in the literature. The second kinematic dynamo problem adopts a spherical shell geometry and non-penetrative and stress-free boundary conditions. The SDDC method will be employed to predict Sunspot cycles.

Buckling analysis and design of thin-walled structures based on novel and intelligent computational methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A REDUCED-ORDER METHOD WITH MIXED NONLINEAR KINEMATICS FOR GEOMETRICALLY NONLINEAR AND BUCKLING ANALYSIS OF THIN-WALLED STRUCTURES

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ABSTRACT

Thin-walled structures subjected to the in-plane and out-of-plane loads are widely used as load-bearing components in the aircraft, space and various civil engineering fields. The out-of-plane deflection of thin-walled structures is normally much larger than the wall thickness when the external load is applied laterally and/or buckling occurs. In these cases, a geometrically nonlinear analysis is required to achieve a realistic load-displacement response which greatly influences the load-carrying capability of thin-walled structures.

The conventional finite element (FE) method with a Newton-Raphson incremental-iterative technique still has limitations for geometrically nonlinear analysis. The repeated linear solutions of a large full-order FE system are computationally expensive, limiting the step size of the path-following analysis. In addition, a sufficient number of path-following steps must be adopted to achieve a geometrically nonlinear response curve with a favorable smoothness. This further aggravates the computational burden of geometrically nonlinear analysis.

In this work, a novel reduced-order method in the framework of mixed nonlinear kinematics is proposed for the geometrically nonlinear analysis of thin-walled structures with large deflections and/or buckling. The mixed nonlinear kinematics are developed in the combination of co-rotational and updated von Kármán formulations. The co-rotational kinematics are used to calculate the internal force and tangent stiffness of the structure, whereas the third- and fourth-order strain energy derivatives are achieved using the updated von Kármán kinematics. For the geometrically nonlinear problem with large deflection, reduced-order models with one degree of freedom are constructed based on the perturbation theory, otherwise more degrees of freedom are involved in the presence of buckling. The use of mixed nonlinear kinematics can greatly improve the computational efficiency in construction of a reduced-order model. The solutions of reduced-order models can be regarded as nonlinear predictors to the geometrically nonlinear response. Nonlinear predictors are required to be corrected using internal force-based residuals to ensure the accuracy of the geometrically nonlinear analysis. A geometrically nonlinear response with favorable smoothness is efficiently and accurately achieved using large step sizes in the path-following analysis. Various numerical examples are applied to validate the numerical accuracy and efficiency of the proposed method.

HINGE AND SMOOTHED-HINGE MODELS FOR CLOTH SIMULATION

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ABSTRACT

The hinge model commonly used in fabric and cloth simulation quantifies bending energy in terms of the angle between the triangular facets defined by four computational nodes with translational but not rotational dofs. The classical hinge model (CHM) starts with the angle between two vectors normal to the triangular facets and derives the first and second order derivatives of the angle for the subsequently nonlinear solution process. In this study, an alternate but an equivalent angle or hinge angle is employed. It leads to the same set of derivatives, but the derivation process appears to be simpler. The torsional stiffness of the hinge is often calculated from the bending energy in one-third or the total area of the two triangular facets which are assumed to be under the cylindrical bending curvature fitting the hinge and the two computational nodes away from the hinge. In this submission, a smoothed-hinge model (SHM) is proposed in which a smooth cylindrical surface is first defined by interpolation at the four computational nodes of the hinge. Under the small curvature and small strain assumptions, the curvatures along the perpendicular directions to the three edges of a triangular facet can be expressed as linear functions of the nodal displacement. The three normal curvatures are transformed into the three curvature components defined in two orthogonal axes on the tangential plane of plate/shell and the conventional bending stiffness matrix used in the plate/shell is used to compute the bending energy. By incorporating the corotational concept, the bending energy can be approximated as a quadratic function of the nodal displacement. As a result, the Hessian of the bending energy is a constant matrix and does not require to be updated in the iterative solution procedure. For the membrane energy, a six-node interpolation instead of the three-node interpolation is employed. The former, when combined with either CHM or SHM, effectively mitigates the occurrence of sharp crease artifacts. To model contact and friction conditions, the incremental potential contact (IPC) is employed. Quasi-static and elasto-dynamic problems are both examined. Through quantitative and qualitative numerical experiments, the results demonstrate that our computational models exhibit stability with large time steps and convincingly simulate a variety of draping and garment scenarios.

Modeling friction and wear
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A GENERAL CONTACT MODEL FOR ROUGH SURFACES BASED ON THE INCREMENTAL CONCEPT

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ABSTRACT

It is now widely accepted that the real contact area between rough solids rises linearly with increasing normal loads. However, the coefficient of proportionality varies among different theoretical models and simulation results. This study advances a model for analyzing the elastic contact of rough solids. By taking into account the specific shape of contacting asperities, the connection between the real contact area and geometric truncation area is established in priority. Furthermore, the relationship between geometric truncation area and normal load is addressed by adopting the incremental concept. For surfaces covered with spherical asperities, the model could reproduce the predictions provided by the celebrated GW model [Greenwood, J. A., and Williamson, J. B. P., 1966, Proc. Roy. Soc. A., 295(1442), 300-319]. Avoiding prescribing the asperity geometries, the model tends to be more robust when surfaces are random and fractal. For general fractal Gaussian random rough surfaces, the model suggests that the coefficient of proportionality lies between 1.67 and 2.56. The upper and lower limits are close to the predictions of the BGT model [Bush, A. W., Gibson, R. D., and Thomas, T. R., 1975, Wear, 35(1), 87-111] and Persson's theory [Persson, B. N. J., 2001, J. Chem. Phys., 115(8), 3840-3861], respectively. In the thermodynamic limit, the potential varying scope for the coefficient of proportionality is further narrowed ranging from 1.92 to 2.22. The resultant predictions are in accord with numerical results presented in literature. The current study might provide profound insights into understanding the role of surface morphologies in elastic rough contact.

Advanced techniques for transport phenomena in heterogenous porous media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL SIMULATION INVESTIGATION ON NONLINEAR FLOW CHARACTERISTICS OF ROUGH SINGLE FRACTURES WITH DIFFERENT CONTACT AREAS

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ABSTRACT

Abstract: To comprehensively understand the influence of the contact area on the flow characteristics of rough single fractures, a rough fracture surface is initially constructed using a spatial frequency domain approach. Subsequently, rough single fractures with varying contact ratios are derived by translating and displacing the fracture surface. The Navier-Stokes equation and Mass-conservation equation are solved by utilizing the laminar flow module integrated within the COMSOL software. The simulation results show that the nonlinear correlation between fluid flow velocity and pressure gradient can be described by using Forchheimer equation. Under the same flow velocity, a higher contact rate will exacerbate the nonlinear characteristics of fluid flow. In contrast to non-contact fractures, the streamlines within contact fractures exhibit increased tortuosity, accompanied by an elongation of flow pathways. Furthermore, with an expanding contact area, the complexity of the streamline pattern amplifies. The overall pressure field distinctly exhibits non-uniform characteristics, with larger pressure gradient observed within localized contact regions, consequently facilitating an increase in flow velocity.

Keywords: Rough fractures; Contact area; Nonlinear flow characteristics; Numerical simulation.

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MULTISCALE MODEL REDUCTION FOR INVERSE HEAT CONDUCTION IN HIGH-CONTRAST MULTISCALE MEDIA

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ABSTRACT

Efficient numerical simulations for forward problems are crucial for decision-making applications like inverse problems and optimal design. However, when dealing with multiscale medium properties, direct numerical simulation of the forward problem becomes computationally expensive, requiring a fine grid to capture variations in highly oscillating material properties. To address this, model reduction techniques are necessary. In this presentation, we introduce a novel multiscale model reduction method for inverse heat conduction in high-contrast multiscale media, significant in various engineering and industrial applications. Our method, grounded in recent advances in multiscale finite element methods, computes multiple localized multiscale basis functions per coarse region using local spectral problems and the localized energy minimization principle. We provide a theoretical analysis of the proposed method and present several numerical tests to verify its performance.

THE EXTENDED MATERIAL POINT METHOD FOR MODELLING EVOLUTION AND INTERACTION OF MULTIPLE DISCONTINUITIES

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ABSTRACT

The Extended Material Point Method (XMPM) has demonstrated efficacy in numerically simulating shear band evolution and post-failure behavior during large deformations. However, the current formulation of XMPM is inherently limited to representing a single discontinuity, constraining its application in modeling intricate scenarios involving multiple discontinuities. This paper introduces a comprehensive extension to the XMPM framework to overcome this limitation, enabling the simulation of realistic problems characterized by the presence of multiple discontinuities.

Our enhanced method incorporates modifications to the original particle displacement approximation, empowering the XMPM to effectively handle multiple discontinuities within the material domain. Additionally, a dedicated contact strategy is developed to deal with the interaction between these multiple discontinuities within the XMPM framework. Several numerical case studies demonstrate the proposed extension's efficacy in simulating scenarios with multiple discontinuities, which is expected to contribute significantly to the understanding and prediction of material failure in various engineering and scientific applications.

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Certification of simulations and model adaptation in computational science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADAPTIVE GRID REFINEMENT FOR HIGH-ORDER FINITE VOLUME SIMULATIONS OF UNSTEADY COMPRESSIBLE AND TURBULENT FLOWS

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ABSTRACT

This study investigates dynamic mesh adaptation (DMA) for hybrid RANS/LES (HRLES) simulations of compressible turbulent flow. HRLES models, which blend Reynolds-Averaged Navier-Stokes (RANS) and Large Eddy Simulation (LES), are by their nature very sensitive to the computational mesh, because of the very different resolution requirements in the RANS and LES regions. The proposed DMA strategy relies on a high-order k-exact finite volume spatial discretization [1] designed to ensure robust, accurate and conservative solutions for compressible flows with strong discontinuities while limiting the numerical dissipation of vortical structures. A mesh refinement criterion related to the truncation error of the k-exact reconstruction scheme is introduced, and compared with several heuristic refinement criteria from the literature [2]. To limit the computational burden of frequent re-meshing for unsteady flow simulations, the adaptation is performed only at certain time steps, and the error criterion is averaged over the chosen adaptation period [3]. A simple and effective criterion is then introduced to automatically control the averaging and adaptation period. The proposed DMA strategy is evaluated against a series of test cases of increasing complexity, ranging from inviscid vortex advection to turbulent transonic flow past an axisymmetric backward-facing step, representative of the base flow behind a space launcher.

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Emerging topology and shape optimization techniques in computational design of materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ANALYTICAL DESIGN SENSITIVITY INFORMATION OF COMPOSITE LAMINATE SHELLS

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ABSTRACT

Fiber-reinforced composites represent a class of materials celebrated for their exceptional strength, lightweight nature, and versatility. These advanced materials are composed of a matrix, often a polymer, reinforced with fibers such as glass, carbon, or aramid. The strategic integration of these fibers provides unique mechanical properties to the composite, combining the high strength of the reinforcing fibers with the flexibility and formability of the matrix material. This synergy results in materials that are widely employed across various industries, ranging from aerospace and automotive engineering to construction and sports equipment manufacturing. The tailored design possibilities and superior performance characteristics of fiber-reinforced composites make them a focal point of research and innovation in materials science and engineering.

In the optimization of laminated composite shells, diverse objective functions are sought depending on the intended use of the structure. This also applies to the selection of design parameters, where, in some cases, alterations in fiber orientations are desired without affecting the thickness of the structure, while in other instances, only specific layer thicknesses, and possibly their fiber orientations, may be subject to variation. This study explores fundamental types of design parameters for composite laminates, including total thickness, specific layer thicknesses, and fiber orientations, with the derivation of sensitivity relations.

Based on the solid shell formulation described in [1], investigations have been conducted for the extension to anisotropic material behavior, cf. [2], and exploring sensitivity relations concerning the shell geometry, cf. [3]. In this work, these methodologies have been used to formulate efficient sensitivity relations of composite shell structures. Employing a variational approach that embeds sensitivity analysis into the continuum mechanical framework, sensitivity relations for layer thicknesses and fiber orientations are established. These continuously derived quantities can be readily discretized and incorporated into a finite element environment.

Numerical examples are referenced to discuss various aspects, such as computational performance, numerical accuracy, and algorithmic treatment.

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A HYBRID VIRTUAL ELEMENT FORMULATION FOR PLANE ELASTICITY

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ABSTRACT

The enhanced Virtual Element Method (VEM) formulation, recently proposed by D'Altri et al. [1] for plane elasticity, provides numerous advantages over the classic VEM. The main innovation resides in the expression of the projection condition through an energy norm in which a divergence-free interpolation is assumed. This leads to the absence of stabilisation terms and a considerable accuracy improvement.
This work shows how the minimisation of Total Potential Energy and the projection operation typical of enhanced VEM can be obtained from the stationarity condition of the Hellinger-Reissner mixed functional. Starting from this theoretical result, a family of polygonal elements for plane elasticity is proposed, named as Hybrid Virtual Element Method (HVEM). The primary unknowns are the displacements along the element contour, as usual in classic VEM, and the stress field. The latter is assumed to within a polynomial basis that a-priori satisfies the equilibrium equations expressed on a Cartesian frame and corresponds to the divergence-free assumption in the projector term in enhanced VEM formulations. Then, all the discrete operators can be evaluated through line integrals, facilitating the formulation for polygonal elements with a generic number of edges [2].
The HVEM not only provides a wider theoretical background, but also reveals a close relationship with mixed hybrid-stress Finite Elements (FEs) [3], traditionally limited to triangular or quadrilateral geometries. Then, leveraging the broad literature on the hybrid-stress FEs behaviour, we discuss the critical role of selecting appropriate stress interpolation functions, not only for the element stability, but also for the accuracy improvement. In particular, a so-called iso-stable interpolation, that adopts the minimum number of stress parameters to ensure the element stability, turns out to be the optimal choice for achieving accurate solutions also for coarse meshes.

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INVESTIGATING EVOLUTION OF VOIDS IN AL2219 USING 3D CHARACTERIZATION AND CRYSTAL PLASTICITY SIMULATIONS

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ABSTRACT

In this work, emerging high-resolution computed tomography (CT) and crystal plasticity (CP) simulations are used to understand void growth mechanisms in aluminum alloy 2219. By combining experimental and computational results, we investigate how microstructural features such as grain boundaries, triple junctions and particles influence void growth. Both DCT (Diffraction Contrasted tomography) and XCT (X-ray Computed Tomography) techniques are used to characterize initial crystal orientations, voids and phases, and their evolution at various applied strains. On the modeling side, high-fidelity crystal plasticity simulations are performed at the same resolution as CT measurements to obtain local stress/strain fields, stress triaxiality and Lode parameter that are frequently used to understand the void growth. Developed framework enables direct and quantitative comparisons between experimental and computational results for understanding void growth mechanisms in metal alloys.

IDENTIFYING CRACKED/DAMAGED STRUCTURES AND THEIR LOCATIONS USING PHYSICS-INFORMED MACHINE LEARNING WITH SPARSE MEASUREMENTS

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ABSTRACT

In this paper, we introduce a novel method for identifying cracked or damaged structures and precisely locating these flaws by integrating physics-informed machine-learning techniques. Our approach combines principles from physics with advanced machine learning algorithms to address longstanding challenges in structural damage detection. By analyzing the vibrational, acoustic, and quasi-static properties of structures, we extract valuable insights from sparse measurement data to detect subtle indicators of structural degradation. Through rigorous experimentation, we validate the effectiveness and precision of our method in detecting structural damage, highlighting its potential to revolutionize current practices in structural health monitoring and maintenance. To demonstrate the performance of the proposed work, several practical examples, such as cracked and damaged structures, were treated. Finally, it was found that the proposed approach is sufficiently accurate despite a few sensor measurement data. It means that it has great potential to evaluate the anomaly detection of large engineering structures.

Mathematics and algorithms for predictive digital twins (DT)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HYBRID SURROGATE MODELING FRAMEWORK AND REINFORCEMENT LEARNING FOR DIGITAL TWIN APPLICATIONS

Jasmin Lim[*1], Dimitrios Pylorof[2], Humberto Garcia[2] and Karthik Duraisamy[1]*

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ABSTRACT

Nuclear energy has high operational risks that a digital twin (DT) can aid in the areas of operations & management (O&M); reactor safety analysis and improvement of plant efficiency. A system surrogate model is developed to predict physical asset quantities (e.g. reactor, heat exchanger, pumps) and computational assets responses (e.g. control system). The system surrogate model is labeled hybrid because it leverages the accuracy of physical models for robustness while also integrating low-fidelity models for speed and predictive capabilities. The framework is applied to a Pebble-Bed Fluoride-Salt-Cooled Reactor (PB-FHR), a new-generation reactor that has drawn interest from both research institutes and commercial companies. The physics-based models are used to compute the relative xenon concentrations and pump degradation, both essential quantities that determine the current reactor conditions. The remaining quantities are predicted using a Vector Autoregressive Moving Average with Exogenous term (VARMAX) model trained with data generated from the System Analysis Module (SAM); a transient system analysis tool for advanced reactor concepts. This model can also update itself by assimilating online measurements. The system state awareness provided by the surrogate model is utilized for the reinforcement learning (RL) of weighing plant operations, predictive maintenance and market performance.

New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION IN MAGNETIC FIELD USING HIGH-FREQUENCY HOMOGENIZATION METHOD

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ABSTRACT

Since the driving performance of a magneto-mechanical system is dominated by the magnetic flux distribution, optimizing the shape of the ferromagnetic material (FM), which determines the path and intensity of the magnetic flux, is the most important design process for improving system performance. The important properties of FMs considered here are the magnetic permeability, which describes the amount of magnetic flux generated due to the magnetic field intensity, as well as the energy loss characteristics due to magnetic hysteresis and eddy currents. In particular, since most magneto-mechanical systems currently under development for industrial devices use alternating electric fields, energy loss occurring within FMs is a critical factor that increases the operating temperature of the system and impairs performances. Therefore, in order to design a high-performance system, it is necessary to use a FM that simultaneously satisfies high permeability, low hysteresis, and low eddy current loss, however it is difficult to develop a new material with these properties.
This study aims to optimize both the microstructure of the FM composite and the shape of the magnetic core using the topology optimization method with a large degree of design freedom [1], and apply the optimized magnetic core with high magnetic permeability and low loss coefficient to a magnetic actuator. To do this, a high-frequency homogenization method, which uses a complex permeability tensor to consider the frequency of the applied magnetic field and predict the eddy current loss density of FMs [2], is applied to magnetic field analysis and design. The optimization problem is formulated to optimize the element density and orientation of the core for achieving the target force and flux distribution, while optimizing the microstructure of the FM that can reduce loss even at high frequency of the applied magnetic field. To verify the effectiveness of the proposed design method, optimized results of a linear oscillatory actuator with high operating frequency are introduced.

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Computational models and methods for predicting cancer progression and treatment response
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PATIENT-SPECIFIC OPTIMIZATION OF THERAPEUTIC REGIMENS VIA DIGITAL TWINS TO IMPROVE TRIPLE NEGATIVE BREAST CANCER RESPONSE TO NEOADJUVANT THERAPY

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ABSTRACT

Neoadjuvant therapy (NAT) is the standard of care for locally advanced triple-negative breast cancer (TNBC). However, pathological complete response (pCR) rate in TNBC patients to current NAT regimens is 50-60% [1]. Aside from the need to develop new therapies with higher efficacy and lower toxicity, a critical barrier to improving TNBC response is the lack of rigorous ways to personally tailor therapeutic regimens. We seek to address this challenge by employing digital twins (i.e., mathematical models that provide a virtual representation of individual patients to predict changes in tumor status) to systematically evaluate TNBC patient's response to different NAT regimens, thereby patient-specifically optimizing treatments.

A cohort of TNBC patients (n = 37) from the ARTEMIS trial (NCT02276433) [2] was used for this study. For each patient, standard-of-care NAT chemotherapy was administered (i.e., 4 cycles of Adriamycin/Cytoxan (A/C) every 2-3 weeks, followed by 12 cycles of weekly Taxol (T)) and longitudinal MRIs were collected before and during NAT. Post-surgical pathology was performed to assess final response status. A digital twin framework has been developed by integrating longitudinal MRIs with a mechanism-based model to predict the treatment response [3]. The model was based on a reaction-diffusion equation that describes the change in tumor cellularity due to migration, proliferation, and drug-induced death. With parameters personalized using the MRIs, the patient-specific model (i.e., digital twin) was used to estimate individual patient's response to 128 simulated but clinically feasible schedules of A/C/T. The predicted response (pCR or non-pCR) from each alternative schedule was compared to the patient response from their actual treatment to evaluate the effect of altering treatment regimens.

We observed that, without changing the total dose, shortening the duration of A/C/T administration increased the treatment efficacy. The effectiveness of altering the schedules varied substantially in different patients. In particular, 8 out of 18 patients who had non-pCR responses to their actual treatment were predicted to achieve pCR with the dense-dose Taxol (i.e., 4 cycles of biweekly Taxol), indicating a 21.62% improvement of pCR rate in the study cohort. We are currently applying the optimization to a larger cohort (n > 130).

The preliminary results of our approach provided a unique opportunity of improving TNBC response to NAT through patient-specific optimization of therapeutic schedules. Ongoing efforts focus on accounting for toxicity and investigating the effects of altering therapy type, dose, and schedule on patient response.

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Computational fluid dynamics (CFD) and fluid-structure interaction (CFSI): Methods and Applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A SIMPLIFIED FLUID STRUCTURE ANALYSIS OF AN ELASTOMERIC SINGLE-LOBE PROGRESSIVE CAVITY PUMP

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ABSTRACT

Widely used in the petroleum industry, progressive/progressing cavity pumps (PCPs) were conceived by René Moineau in the 30s and are in continuous design and efficiency improvement. Notwithstanding, PCPs with an elastomeric stator suffer an efficiency decrease due to elastic deformation provided by the fluid pressure rise along the rotor: in cases with interference, the pressure can cause a clearance, and in cases with clearance, the gap expands. To simulate this phenomenon, the present work improves the model proposed by [1] for the analysis of two-way fluid-structure interaction (FSI) in PCPs, by coupling the element-based finite volume method (EbFVM) for the fluid flow field with more general analytical models for the structural deformation field. The previous simplified structural model was implemented as a FORTRAN subroutine accounting for the local fluid pressure as the structural load in a Hookean linear model for radial deformations only [1]. Although the proposed model can still be considered simplified, it extends the previous one-dimensional structural model to a linear plane stress state considering the Poisson effect, thus making it more realistic. The main goal is to establish a reliable procedure for the development of a three-dimensional structural model for analysis of two-way FSI in PCPs that does not require expensive computational costs, as it is currently required in this type of analysis. The EbFVM was implemented in ANSYS/CFX with a developed FORTRAN code (a DLL routine) for structured mesh generation for each time step analysis accounting for the PCP rotor/stator relative motion [1,2,3]. The results were compared with those obtained with the ANSYS/CFX native mesh deformation algorithm, and with those obtained with the previous one-dimensional approach, showing better accuracy, since the first method causes mesh distortions and hysteresis, whereas the second method does not capture the deformations developed in the angular directions of the stator cross-section.

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Advances in computational biomechanics and mechanobiology
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN EFFICIENT SEMI-ANALYTICAL APPROACH FOR THE STOCHASTIC ANALYSIS OF SOFT BIOLOGICAL STRUCTURES

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ABSTRACT

Introduction: Integration of variability and stochasticity in predictive finite element models of biological systems is of critical importance, particularly in the context of diverse populations, whereby, besides intra-individual variability, there are statistically significant differences in biophysical and microstructural properties across ancestry and age groups. In a mechanobiological context other sources of variability include boundary and loading conditions as well as biochemical factors and their driving forces [1]. Stochastic finite element (SFE) analyses aim to propagate stochastic properties of a system directly through the governing partial differential equations but are more complex to implement and computationally expensive than their deterministic counterparts [2]. It is therefore advantageous to develop general and efficient methodologies to conduct such analyses, especially those that can capture spatial variations of random variables (i.e. stochastic fields).

Method: Here, it is proposed to represent stochastic fields using the Karhunen-Loève (KL) decomposition and calculate the stochastic response of the system using a second-order sensitivity analysis [2, 3]. The numerical implementation, based on automatic differentiation, is general and modular, valid for arbitrary kinematics and constitutive laws, making it particularly attractive to model biological soft tissues and their inherent heterogeneities. KL decomposition is computed via the formulation of a macro-element associated with a Fredholm integral equation of the second kind involving the covariance kernel of the stochastic field, and whose solution is obtained via standard Galerkin procedure.

Results: The SFE framework was assessed on various examples by accounting for geometric and material stochastic fields on 2D geometries, and solutions compared to Monte-Carlo simulations. A path-following method was used to solve the geometrically and materially non-linear problems. The gain in computational speed afforded by the semi-analytical approach could reach four orders of magnitude.

Discussion and Conclusion: The ability of a perturbation approach to capture propagation of uncertainties in highly non-linear systems is inherently limited by the expansion order (here, second order). However, the use of automatic differentiation combined with optimisation of computer code means that extension of the SFE framework to higher orders is possible and should be explored in the future. The numerical framework presented here provides an attractive platform to rapidly and statistically explore the influence of multiple factors on the physics of biological tissues and structures.

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Modeling and simulation of the electro-chemo-thermo-mechanical interactions in energy transition and energy storage systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

QUANTITATIVE NUMERICAL STUDIES OF LITHIUM ELECTROPLATING: VISCOPLASTIC INFILTRATION AND CRACKING IN A SOLID ELECTROLYTE

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ABSTRACT

This talk proposes a mechano–electrochemical multi-phase field (MPF) model to study electroplating in ASSLB, which induces cracking and short–circuiting. Different from previous models [1 - 4], in this model, large viscoplastic deformation is involved to account for huge eigenstrain induced by electroplating; The plating reaction is described by generalized BV equation involving Eshelby stress tensor, which introduces effects of conformational volume change and deformation energy on overpotential; Contact between solid phases is considered to simulate different modes of Li growth associated with mechanical constraint; MPF framework incorporated fracture–PF model to describe cracking and viscoplastic infiltration of Li. Accuracy of proposed model is validated by quantitatively comparing simulated and experimental findings [5].

This model provides a comprehensive depiction of the transition from vertical elongation to shank–expansion of Li whisker for low–voltage plating scenario with variable constraints. It indicates a transition from reaction–controlled root–growth of Li whisker to viscoplastic flow of Li in gaps or cracks. Critical time for transition, depending on bias voltage and stack pressure is quantitatively predicted.

In high–voltage plating with rigid constraints, simulation shows that cracking is caused by wedge-opening mechanism. Specially, if LLZO particle is tightly constrained, Li can only fill in narrow crack via viscoplastic flow rather than pushing sidewalls apart to increase deposition space, quickly resulting in a short circuit. If the LLZO particle is not constrained, the growth of Li changes from the fissure eruption to root–growth that widens the crack and considerably extends short–circuit time. It indicates that reducing mechanical constraints of electrolyte particles instead of increasing their mechanical strength or decreasing defect size can improve cyclability of solid–state battery or mitigate short–circuit.

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Advance and application of meshfree methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INTEGRATING DEEP ENERGY METHODS IN THERMOELASTICITY AND PIEZOELECTRICITY

Kuan-Chung Lin[*1], Kuo-Chou Wang[1] and Cheng-Hung Hu[1]*

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ABSTRACT

This comprehensive study combines two pioneering research works that investigate the use of the deep energy technique for difficult multi-physics issues, especially in thermoelasticity and piezoelectricity. The deep energy approach, which is well-known for its resilience in dealing with nonlinearities and producing exact findings, has been intensively investigated for its efficiency and accuracy in these sectors. The first section of the research looks at its use in thermoelasticity [1], examining how network parameters such as layers, neurons, and activation functions affect result accuracy. Successfully resolving 1D and 2D thermoelasticity issues, which compare favorably with analytical solutions and empirical data, has confirmed this technique. The second portion applies this concept to piezoelectricity [2], solving complex 2D piezoelectric issues as well as piezoelectric composite plate actuators. The tanh activation function emerges as a really useful tool, considerably improving accuracy. This two-part study not only proves that the deep energy method can be used instead of traditional numerical methods to solve multi-physics problems, but it also shows how to set up neural networks in the best way to make them work better and more accurately. This will help both computational physics and engineering.

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Recent advances on interfaces dynamics modeling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STABILITY AND ERROR ANALYSIS OF GENERALISED SAV SCHEMES FOR A DIFFUSE-INTERFACE TUMOUR GROWTH MODEL

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ABSTRACT

In this talk we consider a diffuse-interface (phase-field) model for tumour growth that takes into account nutrient consumption and chemotaxis. The model is described by a nonlinear system consisting of a Cahn-Hilliard-type equation coupled with a reaction-diffusion equation. We first prove the existence of its weak solutions. Efficient schemes are then constructed based on the idea of scalar auxiliary variable (SAV), which we show are not only decoupled and easy to implement, but also have the properties of mass conservation and unconditional energy stability. Furthermore, we derive rigorous error estimates of one of the schemes. Several numerical examples are presented to validate the accuracy and stability of the proposed schemes. It is worth noting that when the scheme is equipped with an adaptive time-stepping strategy, it effciently simulates the typical phenomena of aggregation of multiple tumours with different shapes and tumour chemotactic growth. This is a joint work with Zhaoyang Wang and Junxiang Yang.

Uncertainty quantification and reliability analysis in engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PROBABILISTIC INDOOR NAVIGATION AND OBJECT MANIPULATION OF AUTONOMOUS MOBILE ROBOTS

Po Ting Lin[*1], Shaneza Fatma Rahmadhanty[1], Yu-Chun Huang[1], Ikjin Lee[2] and Kuei-Yuan Chan[3]*

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ABSTRACT

Recently, Autonomous Mobile Robots (AMRs) have become promising solutions for the tasks of picking, transporting and placing objects within dynamic environments in smart factories. AMRs are required to position and navigate themselves within an indoor space that is filled with stationary obstacles such as walls, shelves, tables, machines, etc. as well as moving personnel. Ensuring high precision in the positions and configurations of AMRs is difficult due to factors such as wheel slippage, mechanical part backlash, unstable vibrations, sensor inaccuracies and environmental changes. In this paper, the uncertain motions of a 9-degree-of-freedom AMR (i.e., 3 for the ground vehicle and 6 for the robot arm) have been studied and a probabilistic approach for path and motion planning of AMR has been proposed. The probability that the shortest distance between the AMR and the nearby obstacles exceeds the allowable limit was consistently kept at a safe level. In the optimization process of AMR path and motion planning with obstacle avoidance, a linear probabilistic constraint with respect to the AMR control parameters was utilized to maintain the desired reliability level. In this approach, a Most Probable Target Point (MPTP) was found at the tail of the random distribution of the AMR configuration, which has a shortest distance to a Most Probable Failure Point (MPFP) on the nearby obstacle. Both MPTP and MPFP, which were simultaneously determined by a sub-optimization process, were essential for the formulation of the linear probabilistic constraint. Various numerical examples were utilized to show the performance of the proposed Probabilistic Indoor Navigation and Object Manipulation (PINOM) of AMR.

Multi-scale and machine learning-based modeling methods for optimization and design of composites
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A FAST PREDICTION METHOD FOR BEARING STRENGTH OF AIRCRAFT COMPOSITE BOLTED STRUCTURES CONSIDERING INITIAL ASSEMBLY DEVIATION

Qingyuan Lin[*1], Yong Zhao[1], Yuming Liu[1], Wei Pan[1], Wencai Yu[1] and Yu Ren[1]*

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ABSTRACT

The application of advanced composite materials is currently a key approach to improving the performance of high-end equipment such as aerospace. Joints are the weak points of composite structures. More than 60% of the failure of composite structures occurs in the connection position. Mechanical behavior analysis and joint performance prediction of the assembly and loading process of the composite structure is the key guarantee to realize its expected performance. Bolted joins are the most important form of assembly for composite structures. In the assembly process of composite bolted structures such as airplane wings, due to the influence of the complex multi-source uncertainty factors such as the manufacturing errors of the parts, the accumulation of errors in the pre-procedure assembly process, and the deviation of the assembly tooling, composite laminates always have initial assembly deviations, which are mainly manifested in the shape deviation of the parts and the relative position deviation between the parts. The above shape-position deviations will have a significant impact on the assembly state of the composite bolted joint and result in the joint strength deviating from the design value. This is a key bottleneck in improving the performance of composite bolted structures. Existing related studies have given less consideration to initial assembly deviations, usually focusing on the effect of a single deviation when it acts alone. In fact, there is a significant coupling effect of multi-source shape-position deviations on the assembly results and joint strength. In this study, a fast prediction method for the strength of the composite bolted joints considering the effects of initial shape-position deviation is proposed. This method firstly quantitatively expresses, and data fuses the multi-source initial assembly deviation information of the composite bolted joint. Using the fused deviation information as input, the joint strength is obtained through the virtual assembly-loading analysis. Prepare datasets by parametric sampling and batch simulation. Construct a neural network model and train it using this dataset. Finally, the fast model for the strength prediction considering the initial shape-position deviation of composite bolted joints is established. This model can provide assistance in performance evaluation and calibration of composite bolted joints.

Data science and machine learning applications for composite materials and biomedical engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INVESTIGATING THE EFFECTS OF THE MECHANICAL VENTILATION STRATEGIES ON PULMONARY MECHANICS PROPERTIES FOR CHILDREN WITH ACUTE RESPIRATORY DISTRESS SYNDROME

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ABSTRACT

This study aims to investigate the mechanical ventilator support management and pulmonary physiological characteristics of pediatric patients with Acute Respiratory Distress Syndrome (ARDS) in the Pediatric Intensive Care Unit (PICU).

The lung parenchyma of patients with ARDS often exhibits inhomogeneity, leading to local stress concentration and causing local lung injury, triggering a local inflammatory response. Pulmonary recruitment maneuvers, such as the application of positive end expiratory pressure (PEEP), are common treatments for patients with ARDS. Pulmonary recruitment involves the sustained application of pressure in the airways, allowing collapsed alveoli to reopen. This not only improves oxygenation in patients with ARDS but also helps prevent shear injuries caused by the repetitive opening and closing of alveoli. However, excessive PEEP can also cause lung damage, leading to Ventilator-Induced Lung Injury. At present, the optimal PEEP setting strategy remains unclear and has not yet been determined.

Therefore, we collect ventilator settings records and pulmonary compliance and inflammation evaluation data from patients with ARDS in the PICU. Through data processing and machine learning (including supervised learning and reinforcement learning), we evaluate the impact of different ventilator settings on lung compliance. Additionally, we apply the Ontology Web Language to encode the structural information of respiratory system anatomy and pulmonary mechanics, integrating this information into the machine learning models to enable them to learn from these data. This analysis enhances our understanding of how strategies of mechanical ventilator influence the physiological status of patients, providing more concrete guidance for clinical practices.

UPPER AND LOWER BOUNDS CONFIDENCE BAND COMPUTING FOR ACCURACY AND ERROR ESTIMATION USING SEFEA (STRAIN-ENRICHED FINITE ELEMENT ANALYSIS) FORMULATION

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ABSTRACT

Sefea (Strain-Enriched Finite Element Analysis) formulation[1] has been incorporated into several Industrial CAE products for design analysis for over a decade now. In the latest update, Sefea further refines the enrichment method by incorporating the nodal/element cluster density into the heterogeneous enrichment process. Additional convergence in accuracy is observed even with extremely coarse meshes.

Sefea technology allows general users with minimum or no FEA experience to perform routine design analysis with ease and achieve accurate and robust results. Experienced analysts can leverage speed, accuracy, convenience, and robustness to achieve superior outcomes. As CAD design analysis becomes more prevalent, users are increasingly seeking more guidance on the accuracy and reliability of the analysis results. This is the motivation for the ongoing research.

We first review the Sefea formulation and the critical nature of the zero integral-sum of the enriched strain. The method preserves the constant stress state required for convergence while elevating the low-order constant strain tetrahedron and triangle elements to the 2nd-order element accuracy without additional equations.

We observed that the lower and upper bounds of a given mesh can be derived from the enrichment process in the optimal strain enrichment development[2]. Without any enrichment, the method effectively degenerates into a constant strain low-order element with over-conservative results. Conversely, when uniformly enriched, it exhibits a softened behavior similar to the nodal integration method[3]. In comparison, the proposed enrichment formulation selectively enriches the strain during the integration process based on nodal density, element clustering, and strain variations and produces optimal results within the upper and lower bounds for the given discretization.

The implementation offers a quick feedback on the solution bounds and accuracy with small computational costs by adjusting only the enrichment component without the need for a costly element integral loop. It greatly improves the usability and accuracy projection for general CAE design analysis.

We will present the comparison with the analytical and other numerical methods, evaluating the accuracy, computational efficiency, and general usability. Comparison with traditional error evaluation techniques such as the energy error method is also reviewed. Finally, we highlight the potential areas for future research and development.

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Geometric mechanics formulations and structure-preserving discretizations for continuum mechanics and kinetic models
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DISTRIBUTIONAL COMPLEXES AND THEIR COHOMOLOGY: HESSIAN, DIVDIV, AND ELASTICITY

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ABSTRACT

Recently, there has been a growing interest in discretizing differential complexes beyond the de Rham case, including the Hessian, divdiv, and elasticity complexes. A conforming finite element discretization may involve high polynomial degrees. In contrast, using distributional spaces is much more computationally efficient. Moreover, distributional spaces can be categorized as elements from the dual mesh, which formally establishes a connection between finite element exterior calculus and discrete exterior calculus.

In this talk, I will discuss the distributional Hessian, divdiv, and elasticity complexes and their cohomologies in both 2D and 3D settings. We will prove that the cohomologies are isomorphic to their continuum counterparts. For the Hessian and divdiv complexes, we will first construct the discretization. As for the elasticity complex, we will delve into the Regge complex. Additionally, we will explore the twisted complex of the Regge complex, which can be seen as a differential complex perspective of the microstructure elasticity model.

A HIGHLY PARALLEL SIMULATION OF PATIENT-SPECIFIC HEPATIC FLOWS

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ABSTRACT

Computational hemodynamics is being developed as an alternative approach for assisting clinical diagnosis and treatment planning for liver diseases. The technology is non-invasive, but the computational time could be high when the full geometry of the blood vessels is taken into account. Existing approaches use either one-dimensional model of the artery or simplified three-dimensional tubular geometry in order to reduce the computational time, but the accuracy is sometime compromised, for example, when simulating blood flows in arteries with plaque. In this work, we study a highly parallel method for the transient incompressible Navier-Stokes equations for the simulation of the blood flows in the full three-dimensional patient-specific hepatic artery, portal vein and hepatic vein. As applications, we also simulate the flow in a patient with hepatectomy and calculate the portal pressure gradient. One of the advantages of simulating blood flows in all hepatic vessels is that it provides a direct estimate of the portal pressure gradient, which is a gold standard value to assess the portal hypertension. Moreover, the robustness and scalability of the algorithm are also investigated. A 83% parallel efficiency is achieved for solving a problem with 7 million elements on a supercomputer with more than 1000 processor cores.

Constitutive modeling of complex materials with machine learning and artificial intelligence
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A TWO-STEP CONSTITUTIVE MODELING FRAMEWORK BASED ON DATA-DRIVEN IDENTIFICATON AND PHYSICS-AUGMENTED NEURAL NETWORKS

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ABSTRACT

The formulation and calibration of constitutive models remain a difficult task for materials that exhibit complex nonlinear elastic or inelastic behavior. Therefore, new approaches, generally referred to as data-based or data-driven methods, have become increasingly popular in the computational mechanics community in recent years. However, these approaches require a large amount of data, usually stresses and strains for problems in solid mechanics. In this contribution, we present a consistent two-step approach for the automated calibration of hyperelastic constitutive models which only requires experimentally measurable data.

In the first step of our approach, data-driven identification (DDI) is applied to determine tuples consisting of stress and strain states [1]. This method enables to identify these data by only prescribing the applied boundary conditions and the displacement field which can be determined from full-field measurement methods such as digital image correlation (DIC). In the second step of the proposed framework, the data are used to calibrate a physics-augmented neural network (PANN) [2]. This model fulfills all common conditions of hyperelasticity by construction and is very flexible at the same time. The implementation of the PANN model into a finite element (FE) code is straightforward.

We demonstrate the applicability of our approach by several descriptive examples. Therefore, two-dimensional synthetic data are exemplarily generated by using a reference constitutive model. The calibrated PANN is then applied in three-dimensional FE simulations, where the solution is compared to the reference model.

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BAYESIAN MULTIMODEL INFERENCE IN SYSTEMS BIOLOGY AND MEDICINE

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ABSTRACT

When modeling biological systems, one must often choose from several possible models based on different sets of simplifying assumptions and theories. However, conditioning predictions on a specific model formulation can introduce uncertainty and bias due to the selection of one particular model. Thus, to ensure accurate prediction and uncertainty quantification, we must account for uncertainty in the model formulation in the resulting predictions.

Model selection and discrepancy modeling approaches allow one to choose the “best” model and directly account for model uncertainty. However, given the limited data in many biological applications, these approaches may lead to biases due to the selection of a single model. In this talk, we highlight several methods for multimodel inference that leverage the entire set of available models to avoid selection biases and account for model uncertainty by incorporating contributions from all models. Methods including Bayesian model averaging, pseudo-Bayesian model averaging, and stacking of predictive densities construct robust predictors using the entire model family and avoid conditioning predictions on one model.

In this talk, we characterize multimodel inference with several examples from systems biology, including mitogen-activated protein kinase (MAPK) signaling and prediction of pancreatic function for diabetes diagnosis. Our results show how multimodel inference accounts for model uncertainty and, thus, improves predictive certainty and reduces model selection bias. Furthermore, we demonstrate how multimodel inference yields models that better agree with experimental data and provide more reliable predictions.

Current trends in phase-field modeling and computations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MULTISCALE ANISOTROPIC POLYMER NETWORK MODEL WITH PHASE FIELD FRACTURE AT FINITE STRAINS

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ABSTRACT

This presentation focuses on modeling fracture in rubber-like materials. Our study proposes a multiscale fracture model for elastomers, considering isotropic and anisotropic network responses, using the non-affine microsphere model and the maximal advance path constraint network model, respectively [1,2]. For the latter, macroscale fracture is driven by micromorphic regularization, introducing local-global damage variables. The model is validated using double-edge notched tensile tests and compared with experimental data. Uniaxial tensile experiments on PDMS rubber films with notches are conducted, and simulations are compared with experimental observations. Visualization of stretch and damage evolution in chains oriented differently assesses predictive capacity. Results are compared with alternative models, demonstrating the utility of our approach in accurately simulating rubber-like material fracture behavior.

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Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SOME STRUCTURES PRESERVING KERNEL-BASED METHODS

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ABSTRACT

In this talk, we present innovative kernel-based meshless methods devised to preserve critical structures when solving Hamiltonian and dissipative PDEs. Our first method introduces a conservative Galerkin approach with radial basis functions for Hamiltonian wave equations, ensuring energy conservation through projection operators and a second-order average vector field scheme. The second method details a meshless Galerkin technique for dissipative PDEs on surfaces, which upholds energy dissipation inherently. Both methods are supported by rigorous error and convergence analyses, and their effectiveness is demonstrated with numerical experiments, confirming their theoretical properties.

Constitutive modeling of complex materials with machine learning and artificial intelligence
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ON THE ROLE OF INTERPRETABILITY OF DATA-DRIVEN CONSTITUTIVE MODELING BY CONSTITUTIVE ARTIFICIAL NEURAL NETWORKS

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ABSTRACT

The classical, theory-driven approach to describe the deformation of a material body relies on the formulation of constitutive equations relating strains and stresses. A drawback of this approach are the efforts typically required to develop appropriate functional relations and identify material parameters .

These efforts are not required in data-driven approaches to constitutive modeling. To combine the advantages and overcome the disadvantages of both theory- and data-driven constitutive modeling, we have developed the novel concept of Constitutive Artificial Neural Networks (CANNs). This machine learning approach to data-driven constitutive modeling does not require any major a priori assumptions about the constitutive law but yet incorporates substantial theoretical knowledge about continuum mechanics and constitutive theory. This way, CANNs are able to learn the constitutive law of a material from relatively small amounts of stress-strain data. Moreover, our results suggest that CANNs can robustly discover various flavors of material models from data and by design have clear physical interpretation. These abilities will be illustrated using various data collected from arterial and brain tissue.

New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION APPLIED TO PROBLEMS WITH LOCAL FATIGUE CONSTRAINTS BASED ON AUGMENTED LAGRANGIAN METHOD

Carlos Eduardo Lino[*1], Emilio Carlos Nelli Silva*[1] *and André Luis Ferreira da Silva*[1]

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ABSTRACT

Authors:Carlos Eduardo Lino, André Luis Ferreira da Silva, Emilio Carlos Nelli Silva

Fatigue is the most usual failure mode of any mechanical structure subject to loading. There are several methods to predict the structure life, and different approaches can be applied to extend this life. From the point of view of materials engineering, new materials can be proposed to deal with this issue. However, developing and producing these materials can be expensive. A different approach consists of optimizing the design using some optimization algorithm, determining the optimized material distribution that ensures a higher fatigue life. This work proposes to use topology optimization to design structures subjected to permanent loads to increase the component life. The objective is to minimize the volume, considering fatigue constraints. The works in the literature deal with fatigue constraints using aggregate methods, which are common in problems considering stress constraints. Our proposed approach uses a norm of the stress field to represent the stress constraint. However, stress and fatigue are local phenomena. Thus, in this work, the Augmented Lagrangian method is used to deal with the large number of constraints in the problem. This approach, previously used in stress-constraints problems, makes treating fatigue as a local phenomenon. The Modified Goodman method is used to measure local fatigue. This method considers a sensitivity factor that accurately estimates fatigue life. Numerical examples show the efficiency of the proposed method.

Computational mechanics for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RESIDUAL STRESSES COMPUTATION AND OPTIMIZATION FOR DIRECTED ENERGY DEPOSITION PROCESSES

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ABSTRACT

The adoption of metal additive manufacturing by various industries is being hindered by the presence of residual stresses and distortion in the deposited parts. One of the important challenges that hinder the adoption of metal AM parts is the formation of residual stresses. Layer-by-layer deposition during metal AM causes cyclical heating and cooling of the metal deposit, resulting in the formation of residual stresses [1]. The presence of residual stresses is often undesirable as it could lead to delamination and cracking of deposited parts. Parameter optimization is predominantly used for residual stress mitigation. Finite Element Analysis (FEA) is a valuable tool for predicting residual stresses, but it requires substantial computational power. Direct energy deposition (DED) is a promising additive manufacturing technique that enables the fabrication of complex structures with excellent mechanical properties. This study aims to reduce computational time by incorporating a thermo-mechanical model specifically designed for the DED processes. This model predicts the thermal history and subsequent residual stresses in the deposited material. Various FEA methods are examined to provide a comparative analysis of computational cost and numerical accuracy. These findings contribute towards the realization of a faster modeling approach, where the incorporation of efficient and accurate FEA models can optimize part quality and strength while reducing computational time.

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Numerical modelling of composite materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ELASTIC-PLASTIC SEMI-ANALYTICAL METHOD AND OPTIMIZATION FOR CURVED SCARF BONDING REPAIRS OF COMPOSITE STRUCTURES

Bin Liu[1] and Yancheng Liu*[1]

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ABSTRACT

For the semi-analytical method, Hart-Smith[1] first derived a two-dimensional analysis model for scarf repaired and step repaired isotropic materials. Basing on this method, Harman and Wang[2] introduced average reduction method of composite section elastic modulus, and derived a method for calculating stress distribution of two-dimensional scarf repaired composites. Additionally, they proposed an optimization method to minimize the peak shear stress of adhesive layer by optimizing the bonding angle distribution controlled by first order equation. To restore the stress concentration caused by the change of angles of fiber orientation accurately, Liu[3] improved the method with stiffness-distribution principle and provided a modified analytical method(MAM), which has achieved a more precise and believable result in calculating stress distribution on flat adhesive surfaces. MAM and the application of stiffness-distribution principle has been proven concise effective by Yan[4] with experiments.

In this paper, a semi-analytical stress distribution calculating method that is applicable to arbitrary shape surfaces of scarf repaired composites are proposed. To take not only the cohesive failure caused by shear stress, but also the yield of adhesive under consideration, the adhesive is regarded as an elastic-plastic material. Furthermore, an optimization algorithm basing on this method which could significantly improve the carrying capability of scarf repaired composite laminates is developed. Several examples have revealed high universality and accuracy of this method, and the optimization algorithm developed from which has achieved an excellent effect on reducing peak shear stress. Although it would be difficult to manufacture the optimized surface, this paper still provides a simple but efficient way to evaluate designs of scarf repair and reliable schemes for advancing carrying capacity of scarf repaired composites.

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Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A HIERARCHICAL QUADRATURE ELEMENT METHOD FOR FRACTURE PARAMETERS CALCULATION AND CRACK PROPAGATION SIMULATION

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ABSTRACT

This paper presents a hierarchical quadrature element method (HQEM) with p-convergence for the calculation of fracture mechanical parameters and the simulation of crack propagation with very coarse meshes and high accuracy and efficiency. The stress intensity factor (SIF), strain energy release rate (SERR), J-integral and weight function are computed using minimum mesh refinement and high accuracy. The SERR is directly computed though virtual crack closure method (VCCM) with high accuracy. Although extrapolation is needed in computing SIF and J-integral, they can also be automatically obtained by choosing a certain local mesh size. The computed fracture mechanical parameters are then used to simulate crack propagation using minimum number of elements. The number of elements is significantly reduced through interpolating the crack trajectory as a single curve and modelling the opened crack as two elements only. Thus, the number of elements is unchanged in the whole simulation process, which greatly improves the computational efficiency. The feasibility of applying the HQEM to fracture mechanical parameters computation and crack propagation simulation is demonstrated through several benchmark examples of mode I and mode II fractures (or mixed mode) with homogeneous materials as well as bimaterials. Numerical comparisons with available results in literatures validated the high accuracy and efficiency of the HQEM, which indicates it has promising potential for complex large-scale fracture problems.

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Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SIGNED DISTANCE FIELD ENHANCED VIRTUAL ELEMENT METHOD FOR LARGE DEFORMATION FRICTIONAL CONTACTS IN FLEXIBLE MULTI-BODY SYSTEMS

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ABSTRACT

We propose the signed distance field virtual element method (SDF-VEM), which is a virtual element method variant able to model large deformation frictional contact problems in flexible multi-body systems with signed distance field assisted as a geometrical tool. Leveraging the geometrical versatility inherent in the virtual element method, we could represent each flexible body with either a single-element or a multi-element polygonal mesh of arbitrary shape. This enables node-to-node contact enforcement through adaptive mesh insertion and adjustment. Addressing the complexity of contact detection scenarios in multi-body models, arising from the irregular shapes and numerous bodies involved, we introduce an SDF-assisted unified and automatic contact detection framework. Numerical examples in 2D, including Hertzian contact, spur gears engagements, and granular particles contacts, demonstrate the accuracy and effectiveness of our method.

Multiphysics biomechanics of bio- and bio-inspired soft materials: Theory, simulation and experiments
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GRADIENT-ENHANCED MODELING OF PORO-VISCO-HYPERELASTICITY-INDUCED TIME-DEPENDENT FRACTURE OF BLOOD CLOTS

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ABSTRACT

A blood clot is a natural soft tissue composed of fibrin networks, red blood cells, and platelets. It contributes to hemostasis when it forms on wounded blood vessel walls, while intravascular clots can cause pathological thrombosis. Due to complex physiological loading, their fracture resistance is crucial for physiological hemostasis and pathological thrombosis. However, the mechanism of blood clot fracture is still not well understood. Quantifying blood clots' deformation and fracture is essential for diagnosing and treating bleeding disorders and thrombotic diseases. This work aims to formulate a thermodynamically consistent, multi-physics theoretical framework for describing blood clots' time-dependent deformation and fracture. This theory concurrently incorporates fluid transport through porous fibrin networks, non-linear visco-hyperelastic deformation of the solid skeleton, solid/fluid interactions, mechanical degradation of tissues, gradient enhancement of energy, and protein unfolding of fibrin molecules. The constitutive relations of tissue constituents and the governing equation of fluid transport are derived within the framework of porous media theory by extending non-linear continuum thermodynamics at large strains. A physics-based, compressible network model is developed to describe the mechanical response of the fibrin network of blood clots. The kinetic equations of the internal variables, introduced for describing the non-linear viscoelastic deformation, non-local damage driving force, and protein unfolding, are formulated according to the thermodynamics principles by incorporating a non-equilibrium energy of fibrin networks, a gradient-enhanced energy, and a stretch-induced internal energy of fibrin molecules, respectively, into the total free energy density function. An energy-based damage model is developed to predict the damage and fracture of blood clots. The proposed model is implemented into finite element code by writing subroutines and is experimentally validated using single-edge cracked clot specimens with different constituents. Computational results show that this model can accurately capture the experimentally measured deformation and fracture. The fracture of blood clots subjected to multiple loading conditions is simulated, and the results demonstrate that the deformation and fracture are sensitive to loading rate. The tissue subject to a higher loading rate is stiffer. The damage at the crack tip initiates earlier and propagates faster when the loading time approaches the characteristic time of intrinsic viscoelastic. The fluid transport influences the fracture by tissue swelling. The mechanisms of blood clots fracture are analyzed systematically. The results hypothesize the importance of fibrin network viscoelasticity and fluid transport in the stability of blood clots.

Physics-based data-driven modeling and uncertainty quantification in computational materials science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CORRELATION-BASED LIKELIHOOD-FREE CALIBRATION FOR REALISTIC INVERSION OF MODEL UNCERTAINTY PARAMETERS

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ABSTRACT

The Computational model is widely used to represent physical process property, but the prevalence of uncertainty leads to a failure to match the two. Calibration is often used to tune unknown calibration parameters of a computational model. However, model discrepancy can exist even if all calibration parameters are known. One of the main challenges in model calibration is the difficulty in distinguishing between the effects of calibration parameters versus model discrepancy. Thus, the paper illustrates in detail the reason for the identifiability problem of existing methods, and based on this, we propose a new concept that the computational model and the real physical process should be “the most similar” rather than “the closest”. Further, we propose the correlation-based likelihood-free calibration, which avoids the difficulty of solving the maximum likelihood function while obtaining the most realistic calibration parameters. By comparing all the basic function cases and one common engineering case with the existing methods, the results show that our proposed method can obtain a realistic inversion of the model parameters, and the consistency of the parameters will also significantly improve the prediction accuracy of the model.

Multi-scale, multi-rate damage and fracture: Models, experiments, and simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NOVEL DUCTILE FRACTURE PREDICTION OF ADDITIVE MANUFACTURED TI6AL4V ALLOY

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ABSTRACT

Selective Laser Melting (SLM) is one of the revolutionary additive manufacturing (AM) technologies to produce metallic mechanical parts. To thoroughly understand the damage and fracture behavior of SLM-fabricated Ti6Al4V alloy under complex stress states, the article conducted experimental and simulation studies on various types of Ti6Al4V alloy specimens. By incorporating a novel stress state function into an enhanced GTN (Gurson-Tvergaard-Needleman) model, the study successfully predicted the ductile fracture behavior of the Ti6Al4V alloy.

(1) A number of tensile, compressive and torsional experiments covering various stress states were conducted with different types of the specimens, the study has clearly identified the failure modes under different stress states.

(2) A modified GTN model developed by the Authors' team was adopted in the ductile fracture analysis of SLM-fabricated Ti6Al4V alloy. The introduction of a shear damage variable and a stress state-dependent function extends the application of GTN model to a broader range of stress states.

(3) A parameter calibration strategy of the dual damage variable GTN model was proposed, based on the finite element inverse analysis and referring to a group of experimental results. These parameters encompass quenching parameters and damage parameters, with the latter consisting of 6 parameters related to void volume fraction, 4 parameters related to shear damage, as well as 1 parameter within the stress state function. The applicability of the parameters was well validated via the simulation of another group of experiments.

(4) The morphologies of the fracture surfaces were successfully predicted by using the developed damage constitutive model, and the results demonstrated that the deformation, strength and fracture modes of SLM-fabricated Ti6Al4V alloy can be well described by the developed dual damage variable GTN model. Both damage variables contribute to the different failure mechanisms. The variable of void fraction controls fibrous zone failure based on the void growth mechanism, and the shear damage variable facilitates shear fracture based on the void shear mechanism.

Imaging and computational methods for biomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INCREASED POWER OF HEMODYNAMIC LOW-FREQUENCY OSCILLATIONS CAN IMPROVE CEREBRAL OXYGENATION

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ABSTRACT

Cerebral hemorrhage or ischemia can significantly increase the low-frequency oscillations of blood pressure and cerebral blood flow. Recent studies have shown that such low-frequency oscillations can improve the brain's oxygenation even in the context of reduced cerebral blood flow, which necessitates further investigation. However, this type of study requires special devices, and although previous results have suggested an increase in cerebral oxygenation associated with low-frequency oscillations, it is still unclear whether this increased oxygenation requires a certain power of low-frequency oscillations. We therefore designed and carried out this study.

We recruited 11 healthy subjects aged 18-30 years old, and the experiment was carried out at the Second People's Hospital of Shenzhen. Using the routine clinical syncope test procedure, each participant completed four consecutive stages of the test on a tilt table for syncope testing, including: 10 minutes of supine rest, then the tilt table was raised to a 70-degree angle from the ground within 6 seconds, maintained for 20 minutes, followed by oral administration of 0.25 mg of nitroglycerin, continuing for another 20 minutes, and finally returning to the initial supine position. During the test, we continuously collected blood pressure, bilateral middle cerebral artery blood flow velocity using transcranial Doppler, and near-infrared cerebral blood oxygen signals. Subsequently, we analyzed changes in the power of low-frequency oscillations using power spectral analysis of continuous blood pressure and cerebral blood flow velocity, and calculated changes in the cerebral oxygenation index based on the cerebral oxygen signal.

Our study found that the participants' cerebral blood flow velocity gradually decreased from supine (62.74±1.11 cm/s) to upright (55.65±1.83 cm/s, $P<0.05$) position, and then further after nitroglycerin administration (upright: 55.65±1.83 cm/s vs drug: 43.46±3.93 cm/s, $P<0.05$). At the same time, the power of hemodynamic low-frequency oscillations at approximately 0.1 Hz frequency progressively increased (supine: 45.37±31.38 (cm/s)2Hz-1 vs upright: 133.33±55.71 (cm/s)2Hz-1, $P<0.05$; upright: 133.33±55.71 (cm/s)2Hz-1 vs drug: 243.19±98.82 (cm/s)2Hz-1, $P<0.05$). Interestingly, although the change in cerebral oxygenation index during the upright phase was consistent with the trend of decreasing cerebral blood flow, the cerebral oxygenation index significantly increased when low-frequency oscillations were further enhanced after taking nitroglycerin (upright: 0.0101±0.0008 μM vs drug: 0.0128±0.0008 μM, $P<0.05$).

Therefore, our study suggests that the routine clinical syncope test can effectively induce hemodynamic low-frequency oscillations. We observed for the first time that the increase in cerebral oxygenation index is related to the power of low-frequency oscillations.

Physical models and reduced order models augmentation with data for physics-informed machine learning in real-world applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ENHANCING PREDICTIVE MODELING IN REACTOR BUILDING DOSE DISTRIBUTION: A NEURAL NETWORK-AIDED APPROACH

Jihong Liu[1], Koji Koyamada[1], Hiroaki Natsukawa[1] and Shuhei Kamioka[1]*

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ABSTRACT

Theoretical predictions of dose distribution inside a reactor building using Boltzmann transport equation present a computational challenge due to its substantial resource requirements [1]. To address this issue, we simplify the approach to a diffusion equation in situations where the mean free path of neutrons is relatively short, assuming random scattering [2]. This simplification enhances the manageability of calculations, particularly in scenarios where the scale of computational demands makes Boltzmann equation impractical.

This study involved altering the building shape and radiation source to calculate the Boltzmann transport equation. This methodology enables us to consider various scenarios and conditions influencing neutron transport within the reactor building. The obtained results were then used to derive the diffusion equation through a neural network based on physical information [3]. The incorporation of a neural network introduces computational efficiency and adaptability, thereby improving the practicality of the diffusion equation approach.

The distribution of derivation errors within the building space was visualized, aiding in comprehending the model's accuracy. This visualization highlights areas where the derived diffusion equation may deviate from the more computationally intensive Boltzmann transport equation. The identified regions where the diffusion equation approximation is effective offer valuable insights for practical applications, guiding users on when and where this simplified approach can yield accurate results.

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Advanced materials and smart structures: Modeling, simulation and testing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A CONTINUUM AND COMPUTATIONAL FRAMEWORK FOR NONLINEAR VISCOELASTICITY: BEYOND THE HOLZAPFEL-SIMO APPROACH

Ju Liu[1], Jiashen Guan[1], Chongran Zhao[1] and Jiawei Luo[1]*

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ABSTRACT

Viscoelasticity is a ubiquitous mechanical property in soft matter. The constitutive and computational modeling of nonlinear viscoelasticity is particularly relevant to the understanding and prediction of the performance of various engineering and biomedical materials. There are several desirable features in the design of a model: the soundness in its theoretical root; the potential in accounting for additional materials features (e.g., anisotropy, damage, etc.); the capability to faithfully represent material behavior using as less parameters as possible; the convenience of finite element implementation.

The Holzapfel-Simo model [1] has gained popularity over the past several decades, mainly because it is amenable to finite element implementation and convenient in accounting for material anisotropy. The lack of a thermodynamic foundation has been viewed as a major drawback of this model. In our recent work, we constructed a complete thermomechanical theory for this model and thereby addressed previous concerns [2]. In particular, the study elucidates the origin of the evolution equations of the non-equilibrium stress. It also emphasizes the importance of satisfying the relaxation property for the free energy in the equilibrium limit.

Interestingly, our analysis also reveals that the Holzapfel-Simo model can be regarded as a theory built based on the Green-Naghdi kinematic assumption and the St. Venant-Kirchhoff model for the non-equilibrium elastic behavior. Based on this observation, we extend the Holzapfel-Simo model by incorporating nonlinear effects. A two-parameter strain measure family, which incorporates the well-known Seth-Hill strain family, is introduced. The Green-Naghdi kinematic assumption allows a convenient modular modeling strategy for the inelastic effects using the generalized nonlinear strain measures.

A suite of combined numerical methods is proposed for the computational modeling of the viscoelasticity model. In particular, a smooth generalization of the Taylor-Hood element based on Non-Uniform Rational B-Splines serves as the element technology and is used within a generalized Herrmann mixed variational formulation. A class of strain-drive constitutive integration schemes is discussed, which allows the energy-consistent integration of the overall system. Analysis results and numerical examples will be provided to justify the effectiveness of the proposed methodology.

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Uncertainty quantification and reliability analysis in engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RELIABILITY DESIGN OF MONOPILE FOUNDATIONS IN SPATIALLY VARIABLE SOIL CONSIDERING RANDOM LOADS

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ABSTRACT

Due to the spatial variability of soil properties and the uncertainty of marine environmental loads caused by wind, waves and currents, it is indispensable to perform reliability-based design of monopiles that are extensively utilized in the offshore wind industry. In this study, the random individual capacities and probabilistic VHM failure envelopes of monopiles in spatially variable undrained soil are first obtained using the random finite element method combined with Kriging meta-modelling technique and Monte Carlo simulation. Then, the relationship between the appropriate design (characteristic) quantile of soil shear strength and normalized scale of fluctuation and coefficient of variation of soil strength is investigated when considering the spatial variability of soil as well as the uncertainty of loads. Finally, a design framework of monopiles using appropriate design quantile of soil strength is proposed and verified via an example. The results show that the designed monopile can not only meet the two reliability design requirements set in DNV (2013), but also significantly save costs. The study could be helpful to the design of monopile foundations in practical engineering.

MATHEMATICAL MODELING AND NUMERICAL SIMULATION OF MECHANICAL-THERMAL-CHEMICAL MULTI-FIELD PROCESS

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ABSTRACT

Solid materials are subjected to the interactions of multiple physical and chemical fields when they serve in extreme environments. Their response, such as deformation, mass transfer, heat transfer, and chemical reactions, is intimately related to the failure of structures. Multi-field coupling problems implicate interactions among different physical and chemical fields. Considering the multi-field coupling problem which were affected by the force, heat and chemistry, involves complex dynamic process of multi-component substance in an open system, this work chosen a macroscopically homogeneous body composed of a chemically active medium as the research object. And the force balance, mass balance, and internal energy balance equations were provided based on the fundamental laws of thermodynamics. A fully coupled constitutive model that combines mechanical, thermal, diffusion, and chemical reaction effects was then developed to describe the intricate interplay between these effects. The inertial effects of force, entropy and chemical potential were introduced into a macroscopic uniform body by considering the propagations of elastic waves, temperature waves and diffusion waves. Considering the various influential mechanisms, the contributions of mass diffusion and chemical reaction were separated. The evolution equations of heat conduction, diffusion, and chemical reaction were constructed according to the energy dissipation inequality. This coupling model can effectively describe the transient evolution and quasi-static response of multi-field coupled system. Furthermore, the weak form of governing equations were derived by applying the chemical Gibbs function variational principle, which is based on the universal variational principle of thermodynamics. In particular, the model has the ability in predicting the concentration and entropy jump conditions on the moving interface.
In order to verify the proposed model, the oxidation process of silicon nitride was numerically calculated, and the evolutions of oxide thickness and stress were presented. The results agree with the reference results, indicating that the mechanical-thermal-chemical multi-field coupled model is able to reflect the evolution laws of the stress field, concentration field, temperature field and displacement field of silicon nitride under the coupling effect of multi-physical fields.

Model-based simulations of structural responses under extreme conditions
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NOVEL GPU IMPLEMENTATION OF NONLINEAR EXPLICIT DYNAMIC ANALYSIS FOR COMPLEX CIVIL STRUCTURES

Lanqi Liu[*1], Pu Chen[1], Xianlei Wang[2] and Zhongliang Su[2]*

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ABSTRACT

The explicit integration method is recognized as the main approach for solving nonlinear transient dynamic responses involving material failure and large deformation. Since computation of the explicit integration is intrinsically decoupled, an efficient implement should consider parallel acceleration, especially GPU acceleration. However, there are still some challenges using GPU as the accelerators when large structures contain multiple element types or complex material constitutive models. To this end, this work presents a novel GPU acceleration strategy for explicit integration method for complex structures.

A basic parallelized computational framework is established using the Compute Unified Device Architecture (CUDA). All stages of the explicit dynamic analysis are ported to GPU, including calculating element strains, stresses and internal forces, assembling the nodal effective force and solving the kinetic equations for nodes at every time step. CPU is responsible for data output. Data transfer between the CPU and GPU is necessary only at the output time step. A concurrent execution strategy is designed to solve problems with non-uniformity of element and material types. The FE model is decomposed into a few domains depending on element or material types as well available memory. The aforementioned parallel computing processes for each domain are performed concurrently on GPU. Once the computation of nodal effective forces at each time step of all domains finishes, data communication between different domains is achieved using MPI. Different data for computation mainly reside in global memory, which is the largest memory available on GPU. These data have to be organized in optimal layouts to allow the coalesced memory access. In our data structure, data for elements and nodes are organized in structure-of-arrays. Element matrices with identified size and sparsity in one domain are rearranged as a collection of arrays with each array corresponding to the values at the same matrix position. Additionally, loop unrolling strategy are employed to reduce instruction latency on GPU. Data in one domain are divided into sets with each set of the same size as the thread block. A block with n threads treats p data sets with n entries, each thread handles entries in the same position in p data sets within one execute iteration.
Performance tests from engineering designs show that a speedup of more than 40 is achieved compared to the CPU serial code computing by commercial YJK building software with validated accuracy of the results.

Emerging frontiers and methods in digital manufacturing: Modeling, simulation, and beyond
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MICROSTRUCTURAL CONTROL AND DEFECT ANALYSIS FOR FLOW-MEDIATED CRYSTALLIZATION USING PHYSICS-INFORMED DEEP LEARNING

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ABSTRACT

Crystallization, more generally, liquid-solid phase transitions, is a ubiquitous process of significance for industries ranging from manufacturing to pharmaceuticals. Defect analysis and quality control of crystal microstructure are most important in those processes. To that end, reliable and efficient techniques that can give insight into controlling parameters for achieving desired crystal microstructures are critical. Recently, physics-informed neural networks (PINNs) have shifted the paradigm for scientific computing as a data-efficient computational tool for solving scientific inverse problems.

Based on a novel phase field crystal (PFC) formalism, we will discuss how we construct PINNs to identify key parameters controlling crystallization for systems such as CsPbI_3 perovskites. We will also demonstrate the validation and capability of the inverse problem solver for identifying crystal-level controlling strategies for defect mitigation based on first-principle synthetic data and real experimental data.

Deep and machine learning methodology in the context of application to computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT AND EVALUATION OF MG-CA DEEP LEARNING INTERATOMIC POTENTIALS WITH AID OF AB-INITIO CALCULATIONS

Lijun Liu[1] and Yoji Shibutani*[1]

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ABSTRACT

Key Words: Interatomic Potential, Mg-Ca alloys, First-principles calculations, Molecular dynamics, Deep learning.

Ab initio molecular dynamics (AIMD) has become a significant tool for microscopic understanding of a wide range of problems. However, the spatial and temporal scales that AIMD can access are limited. Most AIMD calculations can only handle systems containing hundreds of atoms on picosecond timescales. On the other hand, conventional molecular dynamics (MD) can be computed efficiently, but its accuracy is limited to empirically determined atomic interaction potentials.

Nanocrystalline structures of metals, which are real-world applications, are composed of tens to hundreds of millions of atoms, which is far beyond the capabilities of ab-initio calculations. However, the main problem with empirical potentials is the need for more accuracy for structures with defects, such as point defects, dislocations, nanoclusters, etc. Therefore, the development of interatomic potentials with high accuracy is crucial.

Recently, some experimental [1] and molecular dynamic results [2] have reported that the ductility of Mg alloys is improved by the solid solution of Ca. In the design of high-performance Mg-Ca alloys, besides the solid solution effect of Ca atoms, the interactions of dislocations, twins, and grain boundaries with microstructures such as Ca solid solution clusters and precipitates are also essential factors to be considered [3]. Most developed Mg-Ca potentials can reproduce some basic properties under an equilibrium state. However, these potentials are not able to give accurate predictions when the state is unstable or defects are included. The present study used datasets from ab-initio calculations to develop Mg-Ca interatomic potentials by deep learning. Our developed Mg-Ca deep potentials can accurately predict not only basic physical, mechanical, and thermal properties but also phase transition under high temperatures and pressures, which is not able to be done by empirical potential.

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Multi-scale, multi-rate damage and fracture: Models, experiments, and simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CREEP LIFE PREDICTION OF COATED TURBINE BLADES CONSIDERING THE INFLUENCE OF FILM COOLING HOLE BLOCKAGE

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ABSTRACT

Blockage of film cooling holes significantly impacts the operational life of coated turbine blades in harsh environments. Understanding the thermo-mechanical behavior of blades under actual film cooling hole blockage conditions is crucial for predicting failure and enhancing reliability. In this study, firstly, blockage morphologies and ratios of all film cooling holes on a full-scale turbine blade were statistically analyzed, leading to the development of a blade model incorporating blockage characteristics. Subsequently, the thermo-mechanical loads of cross-scale membrane-based structures on blades were explored using the shell conduction model and the Chaboche constitutive model. Finally, the Larson-Miller Parameter (LMP) method was adopted as the creep life evaluation criteria, considering both blocked and unblocked scenarios. The results revealed that the blockage degree of film cooling holes was lowest near the leading edge of the blade and gradually increased towards the trailing edge. Additionally, the highest temperature on the blade was located near the blade tip, with the most dangerous zone situated at the root position on the pressure surface. Blockage reduced the surface cooling efficiency and diminished the creep life, increasing the risk of blade failure. In this paper, a calculation method of cross-scale structural life model is proposed to reveal the effect of hole blockage on the creep life of turbine blades, providing valuable insights for durability assessment of coated high-temperature components.

Keywords: Turbine blade; Hole blockage; Thermo-mechanical behavior; LMP method; Creep life

Data science and machine learning applications for composite materials and biomedical engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN EXPLORATION FOR VISCOELASTIC AND DYNAMIC PROPERTY OF 2D CELLULAR MATERIALS

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ABSTRACT

Cellular materials, mimicking natural architectures inside the wood and honeybee’s honeycomb, exhibit a unique combination of high stiffness and low weight. Bridging the gap in prior research on the rate-dependent and the dynamical performance of 2D cellular materials, this study proposes models and explores the viscoelastic behavior and wave propagation of 2D cellular materials. For the viscoelastic property of the material, our study finds that an increase in energy dissipation with rising relative density under strain control but a decrease under stress input. On the other hand, when the angle of cell wall increases, the strong axis of energy dissipation shifts under strain-controlled conditions. Furthermore, the anisotropic feature of energy absorption for auxetic cellular materials is observed. These results highlight the significant effects of microstructure on the viscoelastic performance of 2D cellular materials. In addition, the exploration of dynamical property of the material reveals a remarkable increase in effective Young's modulus and a significant increase in effective natural frequency when the width of cell wall approaches the characteristic material length. This enhancement is pronounced and points out the critical role of size effect in predicting dynamic responses. Moreover, our study indicates that the existence of band gaps in plane wave propagation within 2D cellular materials signifies its inherent ability to suppress energy at specific frequencies. In essence, our exploration offers insights into the intricate relationship between viscoelasticity and dynamic performance in cellular materials, emphasizing the significant influence of microstructure and size effect.

DIGITAL DESIGN OF GRINDING WHEEL FRAME OF GRINDING MACHINE

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ABSTRACT

This research paper explores the grinding wheel holder and feed mechanism to automate the grinding wheel holder. The specific objectives of this research are: (1) Through the determination of the overall programme of the grinding wheel holder of the grinding machine, the disadvantage of low processing efficiency of the ordinary grinding machine is overcome. Through the calculation and verification of the structure, including the lifting beam, serving grinding wheel spindle of the grinder, etc., the design and strength of the parts are verified to be safe and reliable through calculation and verification, and meet the design requirements. Completed the design and selection of the parts, thus improving the machining efficiency and quality of the workpiece. The grinding wheel holder structure is designed to improve the grinding efficiency of the grinding wheel, so that the grinding wheel can work smoothly in the grinder. This structural design extends the service life of the grinder and reduces costs. (2) Finite element analysis and simulation of the parts were carried out to make the structural design of the grinding wheel holder more reasonable, and to improve the reasonableness of the material and structure selection of the grinding wheel holder.

The phase field method for fracture: Theory, numerics, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ASYMPTOTIC HOMOGENIZATION FRAMEWORK FOR PHASE FIELD FRACTURE OF HETEROGENEOUS MATERIALS AND APPLICATION TO TOUGHENING

Sen Liu[*1] and Yongxing Shen*[1]

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ABSTRACT

We propose an asymptotic homogenization framework to account for the fracture of heterogeneous materials. This framework upscales the phase field model for microscale fracture and outputs anisotropic effective properties such as the degraded elasticity tensor and the fracture toughness. Furthermore, it quantitatively accounts for the toughening effect in a succinct way. More specifically, when the critical energy release rate of a heterogeneous material is uniform, the framework reveals that toughening is essentially determined by the disparity of the toughnesses, the energy absorbed by the material before cracking.

New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN INTERFACE-ENRICHED TOPOLOGY OPTIMIZATION FOR MITIGATING THE EFFECT OF SURFACE FLAWS IN 3-D BRITTLE SOLIDS

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ABSTRACT

We propose a fracture-based topology optimization procedure for tailoring the fracture resistance of 3-D brittle solids. Developing on our previous work [1], topology is described by means of a level set function that is parameterized by radial basis functions, and the structural response is computed via the Interface-enriched Generalized Finite Element Method (IGFEM). Semi-circular cracks are assumed to nucleate at the location of enriched nodes that are crated throughout solid boundaries. Energy release rates (ERRs) for all cracks are evaluated by means of topological derivatives, for which we only require the stress field of a single finite element analysis of the uncracked geometry. To that end, an accurate nodal stress field is obtained by means of a non-local stress improvement procedure. The objective function of the topology optimization aggregates all ERRs using the P-mean function. Two schemes are proposed in relation to the direction of cracks: We first fix the crack opening direction to be parallel to either the xz or yz planes. We then relax this restriction and assume the crack opening direction to be perpendicular to the direction of the first principal stress. 3-D numerical examples, including the commonly studied L-bracket benchmark problem, showcase the capability of the procedure.

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TOPOLOGY OPTIMIZATION OF VIBRATING STRUCTURES AND PHONONIC CRYSTALS WITH PRESCRIBED FREQUENCY BANDS

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ABSTRACT

Vibration brings lots of harmful effects for engineering structures in aerospace, high-speed train, and high precision machine, et. al. Thus, how to reduce structural vibration has been a hot topic in engineering and academics. For lots of engineering structures, such as machine tools, vibration isolators, et al., they usually work in some frequency bands[1,2]. When the working or external excitation frequency is equal to or close to the natural frequency of a structure, the resonance phenomenon will happen. Therefore, by reasonably designing the structures and adjusting the natural frequencies to keep away from the common manufacturing or working frequency bands can effectively mitigate the vibration level. In this study, a new continuous and differentiable mathematical formulation of the frequency band constraint[3] based on the modified Heaviside function is proposed to achieve the prescribed frequency bands of vibrating structures. Furthermore, compared to the vibration structural design, the difficulty of phononic crystals' prescribed frequency bands design lies in the correlation between stiffness matrix and wave vector, which is a typical multi-condition eigenvalue problem. Directly utilizing the frequency band constraints may lead to numerical convergence difficulties. Thus the ipsilateral frequency constraint based on a modified Heaviside function is further proposed. Since the developed functions are continuous and differentiable, the sensitivity of the constraint functions can be derived for using the gradient-based optimization solver. The proposed formulation can treat with multi-frequency band constraints and is easily integrated into a topology optimization model. Several numerical examples, including single- frequency band and double-frequency bands problems, are solved by the proposed method. The results validate the effectiveness of the developed method.

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Advanced model order reduction techniques for computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT AND ANALYSIS IN DATA-DRIVEN SYSTEM IDENTIFICATION METHODS WITH APPLICATIONS IN FLUID DYNAMICS

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ABSTRACT

This work will focus on the development and analysis of data-driven system identification methods and applications in fluid dynamics. The objective is aiming to uncover the underlying pattern of the flow based on model-order reduction methods, in addition to the insights of the flow mechanics. The nature of fluid is very intricate mainly because of being nonlinear, immense in spatial-temporal dimensions, sensitive to the boundary conditions and it's interfered by the noise of irrelevant behaviors during the data measurement. The reduced-order models achieve to identify and reconstruct the principal dynamics indicating the physics of the respective flow. In addition, they filter the noise to prevent from the over-fitting problem. The understanding of the nature of fluid dynamics bridges from the broad existence to the numerous applications in diverse fields, such as performance improvement and energy saving in manufacturing which is a priority area in Canada.

Multiphysics biomechanics of bio- and bio-inspired soft materials: Theory, simulation and experiments
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A VISCO-HYPERELASTIC CONSTITUTIVE MODEL OF HYDROGEL BY CONSIDERING CHAIN'S SLIP MECHANISM

Qingsheng Yang[1] and Xinyu Liu[1]*

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ABSTRACT

Polymer is a typical entropic elastic material, and its mechanical response is highly decided by the change of network's conformation. The micro conformation's changing introduces the macro mechanical behavior. For finite deformation, the conformation changes not instantaneously, which leads to visco-hyperelasticity on macro. This process is not only related to loading time but also a multiscale question. In general, the conformation changes in two fields: 1) the single chain's deformation; 2) the relative position's change between chains. To build the bridge from micro to macro, a new transition is put forward in this work. The one-dimensional chain is extended to a three-dimensional cylinder to consider the effect of slippage. Another two free degree is introduced to capture the spatial-temporal characteristic of chain's conformation. The microscopic behavior of chain is then discussed and related to macro behavior of material. The slippage of chain is considered as the main reason leading to the viscosity by this model. This work provides an explanation for the origin of the viscosity in hydrogel by the opinion of chain's motion and gives a new method to build visco-hyperelastic constitutive model.

Advances in computational biomechanics and mechanobiology
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

OPTIMUM DESIGN METHOD FOR ARTIFICIAL EAR OSSICLES BASED ON A HIGH-PRECISION VIBRATION ANALYSIS MODEL

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ABSTRACT

The conductive hearing loss occurs when the middle ear is damaged by various ear diseases, that results in hard sound conduction through the eardrum and three ossicles to the inner ear. The tympanoplasty operation is often carried out to reconstruct the damaged ossicular chain, and to improve the sound conduction efficiency. In the ossicular chain reconstruction, an artificial part called “columella” is produced and used instead of incus which is generally broken. In this operation, the sound conduction efficiency changes by the variations in the shape, material and mounting position of the columella. Currently, the operation is carried out based on the workmanship and experience of the surgeon. In our previous studies, dynamic characteristics of the middle ear in sound conduction have been investigated using three-dimensional finite element method. Based on the analysis results, we have proposed that the hearing restoration effect can be estimated by a comparison of the displacement of the steps footplate between a healthy model and an operation model. Then, designing a reasonable artificial auditory ossicle prior to the operation seems to become possible. However, most of these researches are confined to analytical research dealing with the effect of shapes or mounting positions of the columella, and the optimization based on numerical methods has not been studied.
In the present investigation, an intricate model for the analysis of middle ear vibrations with high precision was formulated, utilizing empirically obtained measurements. A finite element model was also established to simulate the operational dynamics of an impaired ossicular chain induced by chronic otitis media. Subsequently, topology optimization procedures were executed to systematically generate the most optimal configuration for the columella, a pivotal replacement component. The efficacy and soundness of the methodology advanced in this study were substantiated through rigorous verification processes. Notably, the topology optimization of the columella resulted in an augmented vertical displacement of the stapes baseplate, thereby exhibiting potential enhancements in auditory performance post-surgery.

Certification of simulations and model adaptation in computational science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GOAL-ORIENTED ADAPTIVE MULTILEVEL QUASI-MONTE CARLO FOR RANDOM ELLIPTIC PDES

Yang Liu[*1], Joakim Beck[1], Erik von Schwerin[1] and Raul Tempone[12]*

[1]*King Abdullah University of Science and Technology*
[2]*RWTH Aachen University*

ABSTRACT

We present our work titled "Goal-oriented adaptive multilevel quasi-Monte Carlo (MLQMC) for elliptic random PDEs," building upon [Beck, Joakim, et al., "Goal-oriented adaptive finite element multilevel Monte Carlo with convergence rates." Computer Methods in Applied Mechanics and Engineering (2022)] and other ongoing research. Our objective is to solve an elliptic partial differential equation (PDE) with lognormal random input data, when the PDE model faces geometry-induced singularity.

Earlier research [Moon, K-S., et al. "Convergence rates for an adaptive dual weighted residual finite element algorithm." BIT Numerical Mathematics 46.2 (2006)] established convergence rates for a goal-oriented adaptive algorithm. This algorithm utilized isoparametric d-linear quadrilateral finite element approximations and the dual weighted residual error representation in a deterministic context. Notably, this algorithm refines the mesh based on the error's impact on the Quantity of Interest (QoI).

Our current work seeks to merge MLMC/MLQMC with the adaptive finite element solver. Unlike traditional Multilevel Monte Carlo methods, where each sample is determined using a discretization-based numerical method (with resolution tied to the level), our adaptive MLMC (AMLMC) algorithm employs a series of tolerances as its levels. Specifically, for a particular realization of the input coefficient and a set accuracy level, the AMLMC formulates its approximate sample using the initial mesh from the sequence of deterministic, non-uniform meshes. These meshes are produced by the previously mentioned adaptive algorithm and meet the sample-dependent bias constraint. Additionally, the incorporation of QMC enhances the convergence rate.

UQ-TTA student paper competition in uncertainty quantification
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GOAL-ORIENTED ADAPTIVE MULTILEVEL QUASI-MONTE CARLO FOR RANDOM ELLIPTIC PDES

Yang Liu[1], Joakim Beck[1], Erik von Scherwin[1] and Raul Tempone[1]*

[1]*King Abdullah University of Science and Technology*

ABSTRACT

We present our work titled "Goal-oriented adaptive multilevel quasi-Monte Carlo (MLQMC) for elliptic random PDEs," building upon [Beck, Joakim, et al., "Goal-oriented adaptive finite element multilevel Monte Carlo with convergence rates." Computer Methods in Applied Mechanics and Engineering (2022)] and other ongoing research. Our objective is to solve an elliptic partial differential equation (PDE) with lognormal random input data, when the PDE model faces geometry-induced singularity.

Earlier research [Moon, K-S., et al. "Convergence rates for an adaptive dual weighted residual finite element algorithm." BIT Numerical Mathematics 46.2 (2006)] established convergence rates for a goal-oriented adaptive algorithm. This algorithm utilized isoparametric d-linear quadrilateral finite element approximations and the dual weighted residual error representation in a deterministic context. Notably, this algorithm refines the mesh based on the error's impact on the Quantity of Interest (QoI).

Our current work seeks to merge MLMC/MLQMC with the adaptive finite element solver. Unlike traditional Multilevel Monte Carlo methods, where each sample is determined using a discretization-based numerical method (with resolution tied to the level), our adaptive MLMC (AMLMC) algorithm employs a series of tolerances as its levels. Specifically, for a particular realization of the input coefficient and a set accuracy level, the AMLMC formulates its approximate sample using the initial mesh from the sequence of deterministic, non-uniform meshes. These meshes are produced by the previously mentioned adaptive algorithm and meet the sample-dependent bias constraint. Additionally, the incorporation of QMC enhances the convergence rate.

A PHASE-FIELD APPROACH FOR THE NUCLEATION AND PROPAGATION OF DYNAMIC CRACKS

Yangyuanchen Liu[1], Oscar Lopez-Pamies[2] and John Dolbow[1]*

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ABSTRACT

Recently, Kumar et al. [1] proposed and revised a phase-field approach for the nucleation and propagation of fracture under arbitrary quasistatic loading conditions. The model accounts for an arbitrary material strength surface through an external driving force in the evolution equation for the phase-field. In this talk, we extend this model through the addition of inertial forces. The dynamic version of the model is then validated against a broad range of benchmark experiments for dynamic brittle fracture, including the experiments by Kalthoff and Winkler, the Brazilian fracture test, and a recent experiment investigating crack initiation, propagation and branching in soda-lime glass specimens [2]. Numerical simulations illustrate the proposed dynamic phase field model provides reasonable results compared to experimental observations and a cohesive phase field model by Geelen et al [3].

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Boundary element methods: New theories and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SOME ADVANCES ON THE FAST BEM FOR ACOUSTIC PROBLEMS

Yijun Liu[*1], Ruoyan Li[1], Zonglin Li[1] and Zhenyu Gao[1]*

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ABSTRACT

Some progresses on the boundary element method (BEM) for solving acoustic wave problems will be reported in this talk. For the frequency-domain acoustic wave problems, a new fast direct solver is proposed to improve the computational efficiencies in the solutions of the BEM equations. New enriched boundary elements based on the traditional constant elements and using plane wave expansions are also proposed to improve the representation of the variables on the boundary in the discretization of the boundary integral equations. For the 3-D time-domain acoustic wave problems, a new solution strategy based on the concept of a kernel-function library is developed in order to save the computer memory consumption in the solution of the time-domain BEM. Various examples using the above proposed new methods in the acoustic BEM are presented in this talk to show their accuracies and efficiencies in solving acoustic problems in both frequency and time domains.

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Recent advances on interfaces dynamics modeling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NEURAL NETWORKS WITH LOCAL CONVERGING INPUTS (NNLCI) FOR SOLVING CONSERVATION LAWS AND MAXWELL'S EQUATIONS IN VARYING DOMAINS WITH GREATLY REDUCED COMPLEXITY AND TRAINING COSTS

Harris Cobb[1], Haoxiang Huang[1], Hwi Lee[1], Yingjie Liu[1] and Vigor Yang[1]*

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ABSTRACT

This talk is based on a series of joint works (arXiv:2109.09316 and 2204.10424). With Haoxiang Huang and Vigor Yang, we are able to predict discontinuities and smooth parts of solutions of the Euler equations in 1D and 2D by a neural network accurately. For example, in order to predict the solution of the 1D Euler equations at a space-time location, one can design the output of a neural network to be the solution value at the location. If one tries to design the input as the low-cost numerical solution patch in a local domain of dependence of the location (where the information comes from), can the neural network tell if the input is across a shock or in a smooth region ? The answer is no! Our approach uses two numerical solutions of a conservation law from a converging sequence, computed from low-cost numerical schemes, and in a local domain of dependence of a space-time location as the input for a neural network to predict its high-fidelity solution at the location. Despite smeared input solutions, the output provides sharp approximations to solutions containing shocks and contact discontinuities. The method reduces the complexity by several orders of magnitude compared to a fine grid numerical simulation, has much lower cost to train, and can be used naturally in varying computational domains through training and prediction because it's a local method. It can be applied to other differential equations, e.g., the Maxwell's equations for solving electromagnetic waves scattered around complicated PECs (Cobb, Lee and Liu, arXiv:2302.02860).

Multi-scale and machine learning-based modeling methods for optimization and design of composites
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GENERATIVE MODEL TO PREDICT THE DEFORMATION FIELD OF CFRP LAMINATES WITH GEOMETRIC DEVIATIONS IN WING ASSEMBLY

Yuming Liu[*1], Yong Zhao[1], Qingyuan Lin[1], Wei Pan[1], Yu Ren[1] and Wencai Yu[1]*

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ABSTRACT

Thin-walled structure of CFRP laminates is widely utilized in the assembly of aircraft wings. The deformation field generated during the assembly process can impact the assembly performance of the structure, thereby influencing the product quality and operational performance of the wings. The geometric deviations on the critical mating surfaces of the laminate are key factors influencing the deformation fields during the assembly process. Analyzing the mapping relationship between geometric deviations and assembly deformation field plays a crucial role for assessing the assembly results. The traditional analysis methods only consider the impact of simple directional deviations on assembly results and do not comprehensively account for the part geometric deviations. This paper proposes a deviation- deformation analysis framework for CFRP laminates in aircraft wing assembly. The framework introduces a multi-scale geometric deviations modelling method based on the statistical parameters for critical assembly features. Subsequently, it integrates heterogeneous data characterizing shape deviations by employing the encoders. Finite element analysis is then conducted to calculate the assembly deformation field considering the constitutive relationships and damage mechanisms. Taking the parameters representing the geometric deviations as input and deformation field as output, a conditional generative model is employed to learn the influence pattern of the geometric deviations on the deformation field. The framework establishes a prediction model from the deviation field to the deformation field and introduces specific accuracy metrics. Corresponding simulations and experiments demonstrate that the proposed method can predict assembly deformation field more efficiently than traditional numerical methods. It exhibits excellent performance on the accuracy metrics, enabling accurate and efficient field-to-field predictions. This method, by learning expert knowledge such as damage mechanisms and mechanical characteristics during the assembly process, constructs an end-to-end deformation prediction for the CFRP laminates. The predicted results can serve as a research framework for predicting other physical fields.

Machine learning and data driven based engineering computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ANISOTROPIC TAILORED SPINODOID MECHANICAL METAMATERIALS: CONSTITUTIVE MODEL-GUIDED RAPID INVERSE DESIGN AND APPLICATION IN ARTIFICIAL BONE IMPLANTS

Zhanli Liu[*1], Ziming Yan[1] and Zhuo Zhuang[1]*

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ABSTRACT

Spinodoid mechanical metamaterials have garnered significant attention in designing lightweight, high-strength engineering structures and medical implants due to its tunable extreme anisotropic behavior. However, the lack of explicit relationship between complex topology and anisotropic mechanical properties severely restricts rapid inverse design and metal additive manufacturing for spinodoid materials with desired mechanical response. In this study, an integrated methodology leveraging constitutive model-guided rapid inverse design and additive manufacturing for spinodoid metamaterials is developed. First, the volume-fraction- and fabric-tensor-based orthotropic constitutive model for spinodoid materials is developed to describe how topological parameters determine effective mechanical properties. Guided by the parametric constitutive model, representative spinodoid structures are efficiently selected to characterize the mechanical property variation in the whole material space. Next, a deep learning-based model trained by 256 representative spinodoid samples is proposed to inversely design tailored spinodoid materials, which substantially reduces the training sample demand and promotes the pretraining efficiency of design model. Furthermore, by representing the complex 3D spinodoid structure as a two-dimensional topological parameter via dimension reduction method, the explicit structure-property relationship for arbitrary topological parameters is built and the target structure can be efficiently searched by a global optimization strategy. At last, the approach is successfully applied in metal additive manufacturing for tailored spinodoid materials with Ti6Al4V that matches the orthotropic mechanical properties of cancellous bones. The new approach paves an efficient way to build the property-structure-process relationship for precision-engineered spinodoid mechanical metamaterials with tailored mechanical performance in various applications.

Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STABILIZED UNFITTED FINITE ELEMENT METHOD FOR HYDRO-MECHANICAL COUPLING WITH WEAK DISCONTINUITY

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ABSTRACT

The traditional finite element method requires that the mesh must match with various discontinuous, which can significantly increase the difficulty of preprocessing for hydrodynamic coupling problems with complex boundaries and material interfaces. In such case, the finite element method using unfitted mesh is obviously more advantageous, however, this method also has certain problems, for example, irregular mesh cutting may lead to ill-conditioned coefficient matrix to appear, which in turn affects the accuracy and stability of the algorithm. The ghost penalty technique was proposed to overcome the ill-conditioning issue. Recently, an unfitted finite element was proposed for two-field poroelasticity problem, where stabilization terms based on the ghost penalty were developed. Material interfaces are even more difficult to deal with than the boundary as they require careful treatment of the weak discontinuity conditions as well as the mesh cutting stabilization. In this paper, we formulate an unfitted finite element for the poroelastic problem with both material interfaces and complex boundaries. A weak formulation based on the Nitsche's method was developed. Ghost penalty stabilization terms are designed for both sides of the elements intersected by the material interface. The performance of the proposed methodology is tested by several benchmark and practical hydraulic problems of complicated rock-soil mixtures. The numerical results demonstrate optimal convergence rates and low-level condition numbers independent of the mesh cutting.

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Uncertainty quantification and reliability analysis in engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DIMENSION-REDUCTION REPRESENTATION FOR STOCHASTIC GROUND MOTIONS AND ENGINEERING APPLICATIONS

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ABSTRACT

When using frequency domain analysis methods to simulate random seismic actions, both traditional spectral representation and proper orthogonal decomposition belong to the conventional Monte Carlo simulation method. Currently, the conventional Monte Carlo simulation method still face difficulties such as large random variable dimensions, low accuracy of finite simulation samples, and random convergence. To solve these difficulties, this study first derives the original spectral representation (decomposition) of non-stationary random (vector) processes, The sources and significance of classical random amplitude method and random phase method are provided. On this basis, a dimension-reduction representation based on random orthogonal functions is further proposed, which introduces the constraint form of random orthogonal functions to accurately express the full probability information of the random (vector) processes of seismic ground motions with merely several elementary random variables. This dimension-reduction representation has achieved simulation of non-stationary ground motion processes, multi-point and multi-dimensional ground motion vector processes, and continuous ground motion fields. Benefitting from the dimension-reduction representation, each representative sample has assigned probability and all the probabilities constitute a complete set, which lays a solid foundation for the refined analysis of non-linear seismic response and dynamic reliability of engineering structures within the third structural design theory. By far, the dimension-reduction simulation method has been successfully applied to the stochastic dynamic response and overall reliability refinement evaluation of complex engineering structures such as high-rise buildings, large-span bridges, and dams under earthquake action.

Computational mechanics in Canada and China: Current states of shared scientific interests and opportunities for the future cooperation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT AND ANALYSIS OF THE THEORY OF COMPOSITE EXPANSION RING UNDER ELECTROMAGNETIC LOADING

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ABSTRACT

High-speed impact collisions are common mechanical problems in engineering and life. Researchers have recognized that the response of objects under impact loads significantly differs from that under static loads. The dynamic mechanical parameters of materials are crucial for predicting their mechanical response under dynamic loads. Electromagnetic loading expansion ring test technology is essential to achieving a high strain rate tensile loading of materials. The intense pulse Lorentz force is sufficient for low resistivity specimens to achieve the desired strain rate. However, for high resistivity specimens, the induced current is relatively small under achievable loading voltages, making it challenging to obtain satisfactory loading results. Using a low resistivity pusher, the composite expansion ring loading scheme promotes specimen expansion and enables electromagnetic loading expansion ring tests to achieve dynamic tensile loading on most materials. Nevertheless, since this proposed test method, the theory of electromagnetic loading composite expansion rings has yet to develop fully.

This paper comprehensively analyzes the dynamic induction of coil, pusher, and specimen during the process where the pusher promotes the specimen's expansion. It considers the influence of electromagnetic-thermal-mechanical coupling on load results during electromagnetic loading processes and proposes a compound theory capable of accurately predicting composite expansion ring load processes. The simplified compound theory is also presented when dealing with specimens with relatively large resistivities.

The proposed theories in this paper are validated through numerical simulation methods. Furthermore, this paper analyzes the impact of driving ring materials on electromagnetic loading results and investigates how parameters such as coil and capacitance affect electromagnetic loading outcomes. Finally, the applicability of the simplified compound theory is discussed. This paper provides theoretical support for the design of the composite expansion ring under electromagnetic loading.

Constitutive modeling of complex materials with machine learning and artificial intelligence
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VARIATIONAL SYSTEM INFERENCE OF PHASE FIELD FRACTURE MODELS

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ABSTRACT

The mechanical behavior of biological materials is systematically studied in the paradigm of continuum mechanics. Complex phenomena, such as damage and fracture, have been modeled using the phase-field framework in which the total energy functional is minimized with respect to the deformation fields and internal variables (i.e. phase fields) to determine the material's mechanical response [1]. This approach is popular since it can model crack nucleation, propagation, branching, and merging without the need for distinct methods or additional discontinuities in the solution fields. In this work, we present a data-driven inverse method to infer the parameters of a phase-field model of fracture for materials exhibiting complex mechanical responses.

The phase-field fracture formulation has been applied in challenging biological applications such as angioplasty, aneurysm, and ligament tears [2]. This model utilizes hyperelastic free energy that degrades with evolving phase field to model damage and fracture in biological tissues. This general framework takes a modular approach to select a nonlinear stress-strain response and fracture dynamics from a set of hyperelastic models and fracture growth laws, respectively. In our data-driven approach, we identify the best hyperelastic free energy form and damage growth laws from a set of admissible candidates.

We formulate an algebraic optimization problem by considering the weak form of the momentum balance equation with different constitutive models and apply it to the deformation fields. We infer the parameters in the constitutive model and sequentially drop the non-contributing terms to infer the best-suited parsimonious model. This approach is referred to as Variational System Identification [3]. We demonstrate the performance of our methods in the face of noisy data that challenges the identification of mathematical models while attaining high accuracy in the predicted response of the inferred models.

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COMPUTATIONAL MODELING OF MULTILAYERED BENDING PLATES (A 2D+ MULTISCALE APPROACH)

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ABSTRACT

This study introduces a novel 2D multiscale strategy, referred to as the 2D+ approach, employing a computational homogenization formalism tailored for modeling multilayered plates in situations dominated by bending. Such structural elements often involve advanced materials like laminated composites, characterized by a heterogeneous distribution of low-aspect-ratio layers exhibiting substantial nonlinear mechanical behavior across their thickness.

In this methodology, the macroscopic scale is represented by the 2D plate mid-plane, while the mesoscopic scale employs a 1D filament-like Representative Volume Element (RVE) orthogonal to the plate mid-plane, spanning the plate thickness. This RVE captures nonlinear mechanical behavior across the plate thickness at each integration point of the 2D plate discretization. The selected kinematics and discretization at these scales are chosen to effectively capture nonlinear mechanical behavior, achieve computational efficiency, and provide accurate stress distributions compared to high-fidelity 3D simulations.

The proposed strategy aligns with the standard first-order hierarchical multiscale framework, involving the linearization of the macro-scale displacement field along the thickness. It incorporates an additional fluctuating displacement field in the RVE to capture higher-order behavior, computed through a local 1D finite element solution of a Boundary Value Problem (BVP) at the RVE.
A notable feature of the 2D+ approach is the application of the Hill-Mandel principle, establishing mechanical energy equivalence in both macro and meso scales. This weakly couples the 2D macroscopic plate and the set of 1D mesoscopic filaments, resulting in significant computational savings compared to standard 3D modeling. Solving the resulting RVE problem in terms of the fluctuating displacement field enables the enforcement of an additional condition: the fulfillment of linear momentum balance (equilibrium equations). This yields a physically meaningful 2D-like computational setting for the considered structural object (multilayered plates under bending), providing accurate stress distributions typical of full 3D models at the computational cost of 2D models.

DEVELOPMENT, VERIFICATION AND VALIDATION OF 3D FEA-BASED SURROGATE MODELS FOR DAMAGE TOLERANCE APPLICATIONS

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ABSTRACT

The two requirements for a cost-effective modeling procedure in probabilistic fatigue crack growth life assessment are solution accuracy and runtime speed. Quite often, solution accuracy is sacrificed for computational cost using reduced-order models, which can carry some level of solution uncertainty. To overcome such shortcomings, a 3D Finite Element (FE) modeling procedure capable of inserting, analyzing and propagating arbitrary-shaped cracks is employed to generate accurate solutions without the simplifications of geometry, crack shape/path and loading which are associated with reduced-order models.

Since 3D FEM solutions tend to be computationally expensive, machine learning algorithms (surrogate modeling) are used here to leverage the accuracy of the 3D FEM and reduce runtime. Depending on the type of the life assessment requirements, the deterministic solutions consisting of stress intensity factor values, remaining useful life or a 3D crack propagation path, are used for calibrating the surrogate models. The 3D FEA-based surrogate modeling allows for the parametrization of the geometry of interest, loading conditions, crack location, and can be further utilized in probabilistic life assessments. For instance, it can account for intrinsic fatigue crack growth rate scatter as a source of material behavior uncertainty.

Two types of surrogate models suitable for use in probabilistic fatigue crack growth life assessment are developed. For mode I applications, Gaussian Process Regression (GPR) is employed, while for mixed-mode loading cases, where the out-of-plane crack path is a critical output, Radial Basis Function (RBF)-based response surface modeling is utilized. A 3D finite element modeling procedure is used to generate accurate solutions to train the surrogate models, and verification is performed on both types of calibrated surrogate models. Experimental measurements are used to provide validation references for deterministic as well as surrogate modeling solutions.

It was demonstrated that the two surrogate modeling types (GPR and RBF response surface) significantly reduce the solution runtime compared to their deterministic counterparts, making them suitable for probabilistic damage tolerance assessments.

Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMPLEMENTATION OF MICRO-MECHANICAL MODELS FOR MICRO-STRUCTURAL BASED CHARACTERIZATION OF COHESIVE ZONE MODELING (CZM) PARAMETERS FOR DIFFUSION BONDED COMPONENTS

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ABSTRACT

Multilayered aluminum components are of great interest in the aerospace industry due to their high strength-to-weight ratio and corrosion resistance. One of the common production methods of such layered components is diffusion bonding of similar and dissimilar metals. For load bearing applications the bond strength between the different layers is critical. Alongside experimental techniques for assessing bond strength in layered components, a computationally efficient method to model interface failure is the cohesive zone approach (CZM). In this framework the mechanical response of the interface is governed by a traction-separation law (TSL). The TSL represents the relation between the stresses across the interface and the relative displacement between layers, capturing the loss of load-bearing capacity before the final layer separation.

The TSL parameters are commonly determined by fitting of experimental load displacement data and numerical simulations (FEM). In such an approach, micromechanical aspects such as bonding defects (micro-voids) due to oxide layer fracture along the interface, which are known to greatly influence the bond strength, cannot be directly taken into consideration. The goal of the current study is to utilize a micromechanical based FE approach in conjunction with a Continuum Damage Model (CDM) approach to determine the TSL parameters, of diffusively bonded aluminum 7075 specimens, solely based on the defects pattern observed at the interface and a ductile failure law for Al 7075. First the flow-stress of Al7075 at temperatures of 400-500C was determined by cylindrical compression experiments and finite element modelling. Next, Al7075-Al7075 specimen pairs underwent diffusion bonding at 400-500C and thermo-mechanical finite element modelling was used to compute the time dependent thermo-mechanical fields at the specimen interface. Following the bonding experiments, small tensile specimens were cut from the bonded pairs and underwent characterization of the interface using a Scanning Electron Microscope (SEM) and subsequent mechanical testing. The, interfacial morphology observed from the SEM imaging was used to construct microstructural based Representative Area Elements (RAE) of the interface area. To model intact bond failure of the Al7075 in the RAE, a continuum damage approach for Al7075 previously published by the authors was utilized [1]. It is demonstrated that effective TSL can be obtained from the micromechanical models which explicitly take micro-structural parameters of the interface into consideration.

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Current trends in phase-field modeling and computations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN EXTENDED PHASE-FIELD METHOD FOR FRACTURE SIMULATIONS

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ABSTRACT

The extended phase-field method (XPFM) combines the phase-field method for fracture with concepts from the extended/generalized finite element method. The approach aims at a significant reduction of the computational effort in comparison to the standard phase-field method while keeping the advantages of not having to explicitly track the crack geometry and to introduce additional crack propagation criteria.

The XPFM is based on a transformed phase-field ansatz and an enrichment of the displacement field. This allows for much coarser meshes, and it leads to truely mesh independent crack geometries including cracks that run through elements. The transformed phase-field ansatz incorporates knowledge about the analytical solution of the phase-field equation in 1D. The displacement enrichment is entirely based on the phase-field solution, and in contrast to the initial XPFM approach [1], in the present, refined version of the XPFM the necessity to calculate the direction perpendicular to the crack can be avoided completely. This allows for more general applications and the extension of the XPFM to 3D. The displacement enrichment is computed in a discrete way on a subgrid within each enriched finite element on which a phase-field dependent Laplacian problem needs to be solved for each direction. The respective scalar solution fields for the discrete displacement enrichment functions can be obtained in a very efficient way.

In this contribution, the latest developments for the XPFM including the algorithmic treatment will be presented, and applications to common academic examples for the simulation of fracture processes will be shown.

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Modeling, simulation, and AI for ultrasonic NDT and SHM
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NOVEL VARIATIONAL AUTOENCODER ARCHITECTURE FOR TEMPERATURE-ADAPTIVE ULTRASONIC GUIDED WAVE GENERATION

Rafael Junges[1], Luca Lomazzi[1], Lorenzo Miele[1], Marco Giglio[1] and Francesco Cadini[1]*

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ABSTRACT

Ultrasonic guided waves (UGWs) have recently captured the attention of the structural health monitoring (SHM) community. This heightened interest primarily stems from the remarkable sensitivity of UGWs to alterations in the properties of the medium through which they propagate. This makes such waves an interesting diagnostic tool to identify and describe damage affecting thin-walled structures. Among the results of damage diagnosis procedures, anomaly localization is fundamental to drive maintenance actions and restore the health state of the structure. To date, localization has predominantly relied on tomographic algorithms. Despite being widely adopted, they come with unsolved issues, including the generation of artifacts in damage probability maps and the bad performance under varying environmental and operational conditions (EOCs). Consequently, supervised data-driven approaches for UGW-based damage diagnosis have been proposed in the literature. Although such methods are characterized by satisfactory performance, a notable constraint is the requirement for large high-fidelity datasets for training the algorithms, which are typically unavailable for real-life structures. Furthermore, such methods still cannot deal with varying EOCs. A potential remedy lies in unsupervised machine learning methods. These methods have already found application in damage detection within the SHM field, but unsupervised approaches that can localize damage under varying EOCs still have to be investigated in detail. This work aims to overcome the limitations mentioned above by proposing a novel unsupervised network architecture based on variational autoencoders (VAEs). The algorithm was trained over an experimental dataset of UGWs acquired under varying temperature conditions. Testing was performed against experimental signals acquired at temperatures not seen during training to verify that the generative artificial intelligence tool is able to capture the influence of temperature on UGWs.

Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COHESIVE XFEM FORMULATION FOR DUCTILE FRACTURE AT LARGE DEFORMATION

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ABSTRACT

Numerical simulation aided design of large-scale metal and alloy structures under extreme conditions, such as accidental mechanical overloads that may lead to failure, remains a major concern of various industrial sectors such as transportation, energy, and defense.

In this work, we present a three-dimensional numerical approach able to macroscopically account for various dissipative mechanisms (e.g., plasticity and ductile damage) leading to failure. The methodology is developed within the finite strain framework and is implemented into ABAQUS-std finite element computational code as a user finite element (UEL), in view of ensuring mesh-objective results.

Key features of the methodology include its treatment of both geometric and material nonlinearities using an updated Lagrangian formulation (ULF) [1]. The phase of more or less diffuse damage is reproduced by using Gurson-Tvergaard-Needleman (GTN) microporous plasticity model [2] employing standard finite element methods (FEM). Furthermore, the micro-void coalescence phase-induced dilation/shear band is modeled using an innovative extended cohesive finite element approach (XFEM-CZM) [3]. The progressive loss of cohesion culminating in ultimate cracking is addressed with the extended finite elements method (XFEM). A particular attention is paid to transition criteria (damage to localization, localization to cracking), the orientation of the localization plane (especially in Mode II), the cohesive zone model (empirical vs. inspired by the micromechanics of micro-void coalescence), and techniques for overcoming numerical challenges (e.g., volumetric locking [4], numerical integration [5]).

The unified methodology is shown to be able to replicate the degradation process until fracture (progressive drop in resistance, fracture surface orientation) in large elastoplastic deformation of structures used in laboratory tests, even with relatively coarse meshes.

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Contact and interface mechanics: Modeling and computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING SOLID-SOLID CONTACT IN A FULLY EULERIAN PHASE-FIELD FRAMEWORK

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ABSTRACT

This work introduces a novel Eulerian finite element framework based on a phase-field representation of solids to model mechanical contact between elastic solids, with a particular focus on systems involving evolving and intricate surfaces [1]. Traditionally, Lagrangian frameworks dominate in modeling such interactions, yet they often demand sophisticated algorithms for contact detection and resolution. Furthermore, they face difficulties when dealing with solids undergoing dynamic boundary changes, such as crystals growing within confined spaces. Because the physical or chemical evolution demands an Eulerian framework, it is desirable to phrase the mechanical solid boundary value problem in such a framework as well, requiring novel approaches to contact modeling.

Our approach employs the phase-field method that includes a diffuse representation of geometries on a spatial mesh, streamlining the modeling of evolving surfaces. To model elasticity, we make use of the reference map technique [2]. A distinctive feature of our methodology is the introduction of volumetric penalty forces that weakly enforce the contact constraint. Capitalizing on the single reference system, the traction force is defined as a simple function of the phase-fields of the two bodies in contact, which renders contact search obsolete. We demonstrate the validity and versatility of our method through numerical examples, showcasing its capability to accurately capture complex solid-solid interactions.

The Eulerian phase-field formulation significantly simplifies the complexities associated with contact detection and resolution in traditional Lagrangian contact models. Additionally, our framework can be used to seamlessly integrate with other physical phenomena by incorporating multiple energy terms in the evolution of the phase-field. This enables the modeling of multiphysics scenarios, presenting a valuable tool for a broad spectrum of applications involving chemically or physically evolving deformable solids in contact. Such scenarios are, for example, prevalent in deterioration processes of porous media.

In conclusion, our Eulerian finite element framework provides an innovative and promising alternative solution for modeling contact between elastic solids, particularly in scenarios with evolving and intricate surfaces. The methodology's adaptability and capability for multiphysics modeling makes it a promising tool for addressing a wide range of applications, offering insights into the mechanical interactions of deformable solids in contact during processes like growing corrosion precipitates in porous media.

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REDUCED ORDER MODELLING OF EXACT PERIODIC FLOWS USING A SPACE-TIME DISCRETISATION

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ABSTRACT

Periodic flows are omnipresent in a large number of industrial applications. Examples include the flow past wind turbines, rotating flows in turbomachines and the pulsatile flow of blood. Simulation of periodic flows is computationally demanding for design and control applications as they need a long time domain for periodicity in the flow to develop. We circumvent the problem by using a parametric POD-Galerkin reduced order model, which exploits the nature of the problem.

In the full-order model, we apply the framework of residual-based variational-multiscale turbulence modelling and space-time iso-geometric analysis to solve the incompressible Navier-Stokes equations [1]. We convert the initial value problem to a boundary value problem by applying a periodic boundary condition in time to compute the time-periodic states directly. We use the Proper Orthogonal Decomposition (POD) to create a basis using parameter-dependent solutions from the full-order model. The time-periodic basis contains information on space and time, allowing for a dimension reduction in both. We create the reduced-order model using the POD basis and the same stabilisation as the full-order model [2,3]. The reduced-order model can use the DEIM, Q-DEIM and the S-OPT hyper-reduction techniques.

We apply the reduced-order model to flow past periodically heaving and pitching hydrofoils at a Reynolds number of O (103). Parameters include heave amplitude and motion period. The numerical experiments show a fast decay in singular values, allowing for small basis sizes. The results are in agreement with the results of the full-order model.

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Computational models and methods for predicting cancer progression and treatment response
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STRATEGIC INTEGRATION OF PREDICTIVE MODELS: A HOLISTIC APPROACH TO DECIPHERING BREAST CANCER METASTASIS DYNAMICS

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ABSTRACT

In recent years, transformative technological advancements have markedly enhanced our ability to detect individual cancer cells and clusters within patients' blood, lymph nodes, and bone marrow. Despite these groundbreaking developments, the clinical significance of these detected cells remains elusive. This study addresses this uncertainty by introducing a systematic framework designed to select hypotheses that elucidate the population-level dynamics of non- and post-hypoxic cells during breast cancer metastasis to lung tissue. This framework leverages rich data obtained from meticulously conducted ex vivo experiments. Additionally, our approach employs an agent-based model, strategically translating macroscopic information into a microscopic perspective. This enables a comprehensive exploration of dynamic processes and facilitates the generation of novel hypotheses regarding breast cancer metastasis. The efficacy of our framework is demonstrated through the rigorous testing of 1152 candidate models at the population level, resulting in the efficient elimination of unlikely hypotheses and the revelation of valuable insights into the intricate metastatic process. Our multiscale model intricately unravels the proliferative advantage held by non-hypoxic cells within the lung tissue microenvironment. These findings contribute significantly to a deeper understanding of breast cancer metastasis dynamics and bear implications for the development of future therapeutic interventions. This integrated approach serves as a bridge between recent technological breakthroughs and sophisticated modeling techniques, thereby advancing our collective understanding of the complexities inherent in breast cancer metastasis.

Data-enhanced multi-model uncertainty quantification and experimental design of complex computational systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MULTI-FIDELITY APPROACH TO PREDICTION OF FLUTTER BOUNDARY UNDER UNCERTAINTY

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ABSTRACT

We present a multi-fidelity uncertainty quantification (UQ) approach that leverages multiple computational aeroelasticity (CAE) models of various accuracies and costs to characterize the flutter boundary of a wing under uncertainties. The accurate determination of the flutter boundary, which corresponds to the point where the aeroelastic system exhibits zero damping and indicates the onset catastrophic unbounded oscillation, is crucial to aircraft certification. In the presence of model parameter uncertainties, aircraft may experience flutter far below the predicted flutter speed [1]. Our goal is to quantify this uncertainty and to provide the probability of flutter for a range of flight conditions. The problem can be considered a probabilistic extension of the deterministic flutter prediction using multi-fidelity models considered in [2]. Our multi-fidelity UQ approach builds on the following three ingredients: Gaussian process models, which readily incorporate sampled responses from models of various fidelities and provide probabilistic estimates of the damping coefficient over the parameter space; an input-dependent error estimate throughout the parameter space for each model, which is constructed by appealing to the predicted model discrepancies across levels of model fidelities; and contour-targeting adaptive sampling strategies, guided by the expected improvement in and/or estimates of approximation error, to select a sequence of models and sampling points that best improves the approximation of the flutter boundary while accounting for model evaluation costs. We demonstrate the multi-fidelity method for a transonic flutter problem using the following models: a Reynolds-averaged Navier-Stokes CAE model; a Euler CAE; and a traditional aeroelasticity model based on Theodorsen's aerodynamics. The multi-fidelity method enables efficient characterization of the probabilistic flutter boundary and accurately captures the sharp decrease in flutter velocity in the unsteady transonic flow regime with proper model selection.

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EMULATING OCEAN MODELS TO QUANTIFY UNCERTAIN RESPONSES TO CLIMATE CHANGE

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ABSTRACT

To better understand the responses of ocean systems to different forcings that represent climate change scenarios, we have explored a wide range of values for the parameters and initial/boundary conditions in an idealized ocean model on a global scale, NeverWorld2, which has intermediate complexity: it incorporates basin-scale geometry for an idealized Atlantic and Southern ocean, with non-uniform ocean depth to allow for mesoscale eddy interactions with topography. The simulation is implemented in Oceananigans.jl, a Julia-based software package for finite volume simulations of the nonhydrostatic Boussinesq equations on CPUs and GPUs. Due to the complexity of global circulation models, however, simulations of ocean processes are prohibitively expensive (even on GPUs), making the tasks of uncertainty quantification for future predictions and sensitivity analysis for model parameters extremely challenging. To address this challenge, we have investigated a wide range of deep learning tools to build dynamical emulators for targeted quantities of interest (QoIs). In addition, we have explored and developed systematic ways of identifying additional informative or dynamically relevant variables from the governing system, to make these QoI emulators more predictive and accurate. The efficient emulators will make it possible to capture interactions between the ocean and other components of climate models (e.g., atmospheric models, land models, human activities). This provides valuable scientific information for stakeholders in fighting climate change.

The phase field method for fracture: Theory, numerics, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A GENERALIZED FRAMEWORK SUITABLE FOR DYNAMIC AND ELASTIC-PLASTIC CRACK GROWTH PROBLEMS: THE PRINCIPLE OF LEAST EXTERNAL WORK

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ABSTRACT

Starting from the principle of least action, we propose the principle of least external work suitable for dynamic and elastic-plastic crack growth problems. Among those possible crack growth patterns, the principle of least external work indicates that the real one consumes the minimum value of the external work. Like the phase-field method, the proposed principle also converts crack growth problems into an energy minimization value problem, except that the energy term here is the work applied by external loadings. According to the first law of thermodynamics, external work can convert into kinetic energy, elastic and plastic deformation energy, or fracture energy. Therefore, the proposed principle can naturally apply to dynamic and elastoplastic crack growth problems.

Moreover, it can be proved that:
1) For the pure deformation of an elastic solid, the principle of least external work is equivalent to the principle of minimum potential energy;
2) In the case of quasi-static crack growth in elastic solids, the principle of least external work can give the Griffith criterion [1];
3)When a crack grows dynamically in an elastic solid, the principle of least external work can derive the dynamic fracture criterion proposed by Freund [2];
4) When a crack propagates quasi-statically in an elastic-plastic solid, the principle of least external work will give the fracture criterion based on the incremental J-integral [3].

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Battery modeling and computation: From material to device
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTI-PHYSICS SIMULATIONS FOR LI BATTERY

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ABSTRACT

In this talk, I will present some of our recent work of developing battery simulation tools, and how these tools may help facilitate the battery design and management. The prediction of capacity fade and lifetime of batteries is important for cell design, determination of the optimal operation condition and control, and cell maintenance. Various mechanisms contribute to capacity fade. I will talk about a comprehensive capacity fade model and its experimental validation and application for battery optimization; a multiscale approach that couples mechanics and electrochemistry consistently at both particle and electrode scales which enables simulating various electrode phenomena; and approaches to optimize battery health while fulfilling both energy and power requirements. In simulation-based battery design, a large amount of simulations are required to determine the optimal design variables. The computational cost can be prohibitively expensive. I will introduce a new approach of Self-directed Online Learning Optimization (SOLO), which integrates dynamic deep neural network with finite element calculations. SOLO reduces the computational time by up to 5 orders of magnitude compared with directly using heuristic methods, and outperformed all state-of-the-art algorithms tested in our experiments. I will also show a pruner and sampler approach to determine model parameters or battery design parameters, which can reduce the battery testing time by about 75%. Finally, I will discuss simulations of concurrent dendrite and SEI growth.

Computational mechanics of soft matter and machines
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ENHANCING FRACTURE RESISTANCE OF SOFT MATERIALS BY INTRODUCING AN INTERLAYER

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ABSTRACT

Traditional soft materials often experience mechanical failure due to their low fracture resistance, limiting their suitability for various applications. Current approaches to enhance the fracture resistance of soft materials, such as fiber reinforcement and strain-induced crystallization, often involve complex preparation conditions. In this study, we propose a novel and simple strategy to enhance the fracture resistance by introducing an interlayer with lower modulus into the soft material. Through numerical simulation and experimental validation for proposed strategy, it is demonstrated that when a crack crosses the interlayer, the crack driving force decreases significantly and is much lower than that of homogeneous soft materials, thus enhancing the fracture resistance. Furthermore, a crack shielding effect is observed, wherein the material ruptures directly instead of experiencing crack propagation when reaching the stretchability limit, as if the crack were nonexistent. The crack shielding effect can be attained by optimizing both the modulus and width of the interlayer for a specific soft material. The underlying mechanism of this strategy can be explained as the stress de-concentration effect resulting from the introduced interlayer. We hope that this strategy can provide guidance for designing various soft materials with high fracture resistance.

Recent advances in computational fracture mechanics and failure analysis
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADAPTIVE IMPLICIT-EXPLICIT METHOD FOR ROBUST AND EFFICIENT FAILURE ANALYSIS

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ABSTRACT

Although numerous methods have been devised for the failure analysis of quasi-brittle materials, substantial challenges persist in the numerical modeling and simulation of the progressive failure process. Specifically, the damage-induced strain softening may cause convergence difficulty in general implicit procedures, whereas lack of accuracy and restriction on time-step length are problems of concern for explicit formulations. Therefore, investigating and improving the performance of computational models has been of continuing interest within the scientific community.

In the context of continuum damage mechanics (CDM), an adaptive implicit-explicit method (A-IEM) is presented herein to enhance the robustness and efficiency of computational failure models. With standard Newton-Raphson method employed to solve the governing equations (balance of forces), the A-IEM is developed based on a constitutive model for the evolution of damage states. Initially, implicit algorithms are applied for non-linear failure analysis, during which critical nodes that hinder the convergence rate are identified through a concurrent monitoring algorithm. Upon fatal non-convergence, explicit constitutive law is enforced on the corresponding material points to evaluate the damage progression within the current time step. Once the analysis proceeds smoothly, the implicit method is re-activated for subsequent increments. By enabling the seamless transition between implicit and explicit schemes, the proposed A-IEM successfully ameliorates the intrinsic limitations of each standalone method while retaining their respective strengths.

The capability and performance of the proposed A-IEM are demonstrated through several representative benchmark problems. The progressive failure process of quasi-brittle materials is studied, where both A-IEM and conventional finite element schemes are applied for model comparison. The first example presents curved crack growth in an L-shaped plate while the second example considers a single-edge notched beam subjected to three-point bending load. To further validate the model adaptability, the anisotropic CDM is incorporated into the A-IEM framework, allowing for the failure analysis of a composite laminate in the last example.

PHYSICAL-BASED ESTIMATION OF INTER-SECTION BRIDGE RESPONSES UNDER VEHICULAR LOADING WITH BP-ANN

Xuzhao Lu[*1], Limin Sun[1], Ye Xia[1], Guang Qu[1] and Haibin Sun[1]*

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ABSTRACT

Estimation of inter-section bridge responses is a developing technique for monitoring bridge health. Monitoring data is used to estimate bridge responses at specific cross-sections by comparing them to responses at other cross-sections. These estimated responses serve as a baseline for comparison with the monitoring data. If significant differences are observed, it is possible that structural damage has occurred on the bridge.

Previous research has typically classified inter-section response estimation as a time-series prediction problem. To solve this problem, popular machine learning methods such as long-short-term memory (LSTM), convolution neural network (CNN), and transformer have been utilized. However, these methods primarily focus on time-dependent characteristics, including seasonal tendencies, yearly tendencies, and other periodic regulations. However, this paper demonstrates that the relationship between inter-section responses is essentially a time-independent mapping. The use of the aforementioned methods may lead to overfitting.

This paper analyzes the theoretical physical dynamics of a typical vehicle-bridge-interaction (VBI) system based on the derivation of dynamic equations. The inter-sensor relationship is represented as a transform determined by model shapes, which is proved to be time-independent. Then, the BP-ANN method is utilized for inter-sensor response estimation. The proposed method was validated using field monitoring data from a concrete bridge. Firstly, the dynamic responses of the bridge were separated into high-frequency responses and low-frequency driving-force related responses. Then, the BP-ANN was applied to each component. Responses from multiple sensors at certain cross-sections were used to predict the responses at a specific cross-section. The estimation results matched well with the monitoring data. Moreover, we proposed a comparison between the BP-ANN and other time-series prediction methods. Our findings indicate that the BP-ANN can effectively avoid over-fitting problems. Furthermore, our study demonstrates the potential for using small-scale monitoring data for long-term health monitoring, including temperature and traffic conditions. This approach can be widely applied in actual engineering.

Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXTENDED TENSOR DECOMPOSITION MODEL REDUCTION METHOD: APPLICATION TO ADDITIVE MANUFACTURING RESIDUAL STRESS PREDICTIONS AND UNCERTAINTY QUANTIFICATION

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ABSTRACT

Simulation-based science and engineering, including design and uncertainty quantification, usually necessitate fast responses of numerical models. Despite the significant improvement of the computer hardware over the last decades, real-time simulations of large-scale systems are still intractable with conventional finite element analysis (FEA). The repetitive evaluation of the numerical model using FEA makes the design process computationally prohibitive.

This work presents an eXtended Tensor Decomposition (XTD) method [1] for nonlinear model reduction. The XTD method is based on a sparse non-separated enrichment to the conventional tensor decomposition [2,3], which can improve the approximation accuracy and the reducibility (compressibility) in highly nonlinear and singular cases. The method has been successfully applied to parametric elastic–plastic problems for real time additive manufacturing residual stress predictions with uncertainty quantification. The efficiency of the method is demonstrated with comparison to full-order FEA. The proposed method enables a novel computational framework for fast manufacturing process design with uncertainties.

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A NEW NONLINEAR SHELL FINITE ELEMENT WITH A CONSERVATIVE DYNAMIC ALGORITHM

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ABSTRACT

The exploration of shell simulation within the Finite Element Method (FEM) carries significant importance in the field of structural engineering and dynamic analysis, particularly when dealing with structures exhibiting considerable displacements, such as wind turbine blades. However, simulating extremely thin structures using prevalent commercial finite element software often encounters numerical limitations. These challenges typically manifest as the artificial numerical stiffness of the shell at the finite element level, commonly known as locking phenomena, or the use of non-conservative numerical schemes that fail to maintain energy and/or momentum conservation, resulting in unrealistic outcomes.

In response to these issues, the current research aims to introduce a novel FEM model that prioritizes simplicity and conservative dynamics. Building upon previous work conducted by our research group (refer to [1~5] for examples), our ongoing investigation focuses on implementing a new conservative finite element capable of simulating thin nonlinear shells in long-term dynamic boundary value problems.

This innovative element, featuring six nodes, employs a unique scheme with a non-conforming rotational field constructed from an incremental rotation variable φ_Δ (introduced in [1] by our group). This approach eliminates the need for employing numerical techniques like penalties, Lagrange multipliers, or any other artificial parameters to address C1 continuity—a kinematic requirement for Kirchhoff-Love shell theory. The standard six parameters representing the quadratic displacement field of the mid-plane are incorporated at the element's six nodes. The dynamic algorithm is rooted in previous work by [2], specifically developed for energy and momentum-conserving simulations of rod and shell finite elements. This algorithm is proficient in handling rotational degrees of freedom and general hyperelasticity.

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Recent advances in meshfree and particle methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE CHOICE OF THE SHAPE PARAMETER IN THE SHIFTED SURFACE SPLINE

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ABSTRACT

Abstract. This is a continuation of our previous study of the shape parameter contained in the shifted surface spline. We insist that the data points be purely scattered without meshes and the domain can be of any shape when making function interpolation by shifted surface splines. We also endeavour to make our approach easily accessible for scientists, not only mathematicians. However, the space of interpolated functions is smaller than the one used before, leading to sharper function approximation. This function space has particular significance in numerical partial differential equations, especially for equations whose solutions lie in Sobolev space. Although Fourier transform is deeply involved, scientists without background for Fourier analysis can easily understand and use our approach.

Advances in damage & fracture modeling of multiphysics materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THERMOMECHANICAL FATIGUE IN HIGH TEMPERATURE STRUCTURES: DEFORMATION BEHAVIOR, DAMAGE MODELING AND LIFE PREDICTION

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ABSTRACT

Nickel-base single crystal superalloys (NBSX) are widely used in turbine blades of aero engines. As a multi-physics problem, thermomechanical fatigue (TMF) is considered to be a key factor limiting the safe service of hot-end components. Mechanical fatigue, thermal-induced creep and oxidation at elevated temperature are involved in TMF. It is important to model TMF damage and failure for structural integrity and strength design of engines.

In this study, TMF tests were conducted on both standard smooth specimens and film cooling hole (FCH) structure of DD6 alloy, including IP and OP loading paths. It was found that the fatigue life of TMF decreased by 90%-98% compared with the isothermal fatigue life at the same peak cycle temperature.

Secondly, damage mechanisms were revealed by microscopic characterization of fracture surfaces. Creep damage and fatigue damage dominated in IP-TMF. The effects of slip system on damage development and accumulation were discussed. In OP-TMF, oxidation assisted both fatigue crack nucleation and propagation. In the FCH structure, it was unveiled that stress concentration and stress ratio had tremendous impact on damage mechanisms. Transition from mode I to crystallographic fracture was captured.

Then, a novel crystal plasticity constitutive model was developed for TMF deformation behavior of NBSX. The influences of temperature on the elastic-plastic parameters and the activation of different crystallographic slip systems were considered. FEM simulation was conducted and stress-strain responses on various crystal orientations were well modelled. Local deformation around the FCH was simulated and verified by digital image correlation (DIC) method.

Finally, anisotropic fatigue damage and creep damage were modelled along slip systems based on continuum mechanics. The models were verified by isothermal low-cycle fatigue, pure creep and creep-fatigue test results. The oxidation damage was quantified by the thickness of the oxide layer. Based on the linear damage accumulation rule, a novel anisotropic TMF life prediction model was proposed. The effect of stress concentration on TMF life was incorporated. Experimental data of both smooth specimens under different crystal orientations and FCH structure were evaluated and most of the lifetime points fell within the 2-time scatter band.

Aiming at the TMF problem of hot-end structure, a systematic study of high temperature tests-mechanism analysis-deformation simulation-damage modeling-life prediction was conducted in this work. This study highlights how crystal anisotropy, stress concentration and loading paths affect deformation and various damage mechanisms, providing key insights into constitutive and damage modeling of high temperature structures under TMF conditions.

Advances in multi-scale, multi-material, and multi-component Topology Optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BI-DIRECTIONAL FIBER ORIENTATION DESIGN FOR MANUFACTURING IN FIBER-REINFORCED COMPOSITES

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ABSTRACT

Optimizing continuous fiber orientation is crucial for designing fiber-reinforced composite structures, especially when employing advanced manufacturing techniques such as automated fiber placement and additive manufacturing. While existing studies effectively capture the bi-directional mechanical properties of fibers in the constitutive models, i.e., a fiber has same mechanical properties in the fiber direction and its opposite direction, representing their bi-directional geometric properties is often overlooked by traditional orientation representations. This oversight can impact manufacturing evaluations, as constraints vary when fiber orientation is flipped. The present work aims to address the following two key questions: first, can we represent the bi-directional properties of fiber orientations both mechanically and geometrically? Second, if achievable, how can we enhance design manufacturability under such bi-directional orientation representation to overcome limitations in the current design space?

The proposed methodology is applied to optimize compliance in 2D plates and 3D shell structures with continuous fiber paths. The design process integrates a thorough assessment and management of critical manufacturing constraints, encompassing both the minimum turning radius of fiber paths and the maximum density of gaps/overlaps. Numerical results demonstrate enhanced structural performance and effective control over design manufacturability through the bi-directional fiber orientation design for manufacturing in fiber-reinforced composites.

Multiphysics and data-driven modeling for cardiovascular biomedicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SHAPE OPTIMIZATION OF A GEOMETRICALLY-ADAPTABLE HEART-VALVED CONDUIT FOR PEDIATRIC APPLICATIONS

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ABSTRACT

Congenital heart valve disease in pediatric patients necessitates using prosthetic valves, yet conventional valves struggle to sustain optimal hemodynamic performance as the vascular system grows. The dynamic nature of infant cardiovascular development, where the valve diameter can double due to somatic growth, often leads to multiple replacements before adulthood, requiring high-risk open-heart surgeries. Overcoming this challenge involves the development of an adaptable heart valve with an optimized geometry capable of maintaining excellent cardiovascular performance across different growth stages. Here, we introduce an optimization framework for designing expandable bi- and tri-leaflet valved conduits. The leaflet shapes, represented by Bezier curves and other sizing parameters, are incorporated into a computer-aided design (CAD) model. The valve's closing and opening processes are modeled with physiologically relevant boundary conditions across three stages: pre-dilation, dilation, and post-dilation. The anisotropy of the polymeric material used for the valve is rigorously characterized through uniaxial tension tests and represented using anisotropic elastic-plastic material models. All the simulations are performed using a quasi-static finite element analysis (FEA) in LS-DYNA. During the iterative updates of the design variables, the CAD and the FEA models of the valved conduit with varying geometries are automatically generated. The objective is to minimize maximum principal stresses, plastic strain, and orifice area ratios in both pre-dilation and post-dilation performance evaluations. Genetic algorithms (GA) are employed to solve the multi-objective optimization problem, yielding a set of Pareto solutions. From this set, an optimized design is selected in the decision-making process. Subsequently, fluid-structure interaction (FSI) simulations are conducted to assess the performance of the optimized heart valve, ensuring its functionality in a physiological setting. This comprehensive approach aims to advance the design and development of prosthetic heart valves capable of adapting to pediatric patients' evolving cardiovascular needs, ultimately reducing the need for frequent surgical replacements and mitigating the associated risks.

Advances in neural operators for scientific modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFICIENT PDE-CONSTRAINED OPTIMIZATION UNDER UNCERTAINTY USING DERIVATIVE-INFORMED NEURAL OPERATORS

Dingcheng Luo[*1], Thomas O'Leary-Roseberry[1], Peng Chen[2] and Omar Ghattas[1]*

[1]The University of Texas at Austin
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ABSTRACT

We propose a novel machine-learning framework for solving optimization problems governed by partial differential equations (PDEs) with high-dimensional random parameters [1]. Such problems arise, for example, in the design of structures with uncertain material parameters/loads and the control of fluids under uncertain flow conditions. Optimization under uncertainty (OUU) is often orders of magnitude more computationally intensive compared to its deterministic counterpart due to the need to estimate the risk-based objective functions by stochastic integration. This requires numerous solutions of the governing PDE at every optimization iteration, potentially amounting to prohibitive computational costs.

To address this challenge, we consider a derivative-informed neural operator (DINO) [2] that approximates the solution operator of the PDE, mapping from the joint inputs of the random parameters and optimization variables to the PDE solution. In particular, we propose to incorporate the derivative of the PDE solution operator with respect to the optimization variables into the training loss. The additional information provided by the derivatives ensures that both the optimization objective function and its gradients can be simultaneously approximated to high accuracy with only a limited number of training samples, leading to more accurate OUU solutions.

We demonstrate the accuracy and efficiency of our approach through several numerical experiments of flow control problems in two and three spatial dimensions subject to random field inputs. Across the examples, the DINOs offer 3–7 orders of magnitude reductions in execution time. Moreover, the DINOs can produce OUU solutions of comparable accuracies to those from standard PDE-based solutions while being 10–100× more cost-efficient, even after factoring in the cost of training data generation.

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UQ-TTA student paper competition in uncertainty quantification
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFICIENT PDE-CONSTRAINED OPTIMIZATION UNDER UNCERTAINTY USING DERIVATIVE-INFORMED NEURAL OPERATORS

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ABSTRACT

We propose a novel machine-learning framework for solving optimization problems governed by partial differential equations (PDEs) with high-dimensional random parameters [1]. Such problems arise, for example, in the design of structures with uncertain material parameters/loads and the control of fluids under uncertain flow conditions. Optimization under uncertainty (OUU) is often orders of magnitude more computationally intensive compared to its deterministic counterpart due to the need to estimate the risk-based objective functions by stochastic integration. This requires numerous solutions of the governing PDE at every optimization iteration, potentially amounting to prohibitive computational costs.

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Minisymposium in honor of Prof. Yannis Kallinderis's 60th birthday: Progress of Unstructured grid based CFD, hybrid mesh generation and adaptation, and parallel supercomputing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPLORING INTERFACE CONSERVATION IN COMPUTATIONAL FLUID DYNAMICS

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ABSTRACT

The necessity of enforcing conservation in computational elements or cells (element conservation) for discontinuous solutions is well understood and respected for solving conservation laws in computational fluid dynamics (CFD). In contrast, interface conservation, where the conservation across cell interfaces is enforced is long ignored, and yet is also ruled and required by the underlying physics just like element conservation. Violation of the interface conservation across discontinuities is the root cause why an exact discontinuous solution can never be achieved in shock capturing methods. The interface conservation is examined and explored thoroughly in this paper. A discontinuity indicator based on the interface conservation is developed to reliably detect and identify all types of discontinuities, as the interface conservation can never be attained across the discontinuities. The developed discontinuity indicator is used as an error indicator for h-adaptive grid methods to effectively increase mesh resolution near discontinuities and for r-adaptive grid methods to align mesh interfaces with discontinuities using a moving discontinuous Galerkin (MDG) Method. A number of numerical experiments are conducted to assess effectiveness of the interface conservation-based error indicator and performance of the MDG method. Numerical results for a variety of discontinuous flows obtained indicate that the error indicator based on the interface conservation can effectively detect all types of discontinuities and under-resolved flow regions and the MDG method by enforcing the interface conservation is able to reposition grid, align mesh interfaces with all types of discontinuities, and achieve the designed order of both h- and p-convergence even for discontinuous solutions.

Imaging and computational methods for biomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INEXACT NEWTON WITH LEARNING-BASED PRECONDITIONER FOR HIGHLY NONLINEAR HYPERELASTICITY PROBLEMS ON THREE-DIMENSIONAL UNSTRUCTURED MESHES

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ABSTRACT

Inexact Newton-type method is widely used in many scientific and engineering applications, but in many situations it converges slowly or even fails to converge, for reasons that are difficult to quantify. We propose a novel nonlinearly preconditioned inexact Newton algorithm with learning capability to improve the convergence and robustness of the method. The proposed method searches through the nonlinear residual and stagnated solution spaces generated during the Newton iterations and identifies the "bad subspaces" using an unsupervised learning technique, namely principal component analysis. In the nonlinear preconditioner, a learned small-scale projected problem corresponding to the slow subspace of the nonlinear residuals is constructed and solved to provide a much better initial guess for the global inexact Newton method to converge nearly quadratically. As an application, we consider the modeling of the human artery with stenosis using the hyperelasticity equation with multiple material parameters. Due to the significant difference in the material coefficients between the plaques and the healthy parts of the blood vessels, the problem is nonlinearly very difficult. Numerical experiments demonstrate that the proposed nonlinearly preconditioned inexact Newton offers significantly reduced number of nonlinear iterations and robustness for this rather challenging hyperelasticity problem.

Computational mechanics in high-strain rate and impact engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DISLOCATION DYNAMICS IN TANTALUM UNDER LASER SHOCK: ELUCIDATING THE CRITICAL ROLE OF ELASTODYNAMICS EFFECTS

Shichao Luo[*1] and Yinan Cui[1]*

[1]*Tsinghua University*

ABSTRACT

This report explores the significant role of dislocation elastodynamics in shaping the plastic behavior of metals under the extreme conditions of intense laser shock, with an emphasis on tantalum single crystal. It critically evaluates the shortcomings of conventional dislocation dynamics methods, which rely on elastostatics theory and often fail to adequately address the intricate spatio-temporal coupling effects manifesting in various dislocation velocities—ranging from subsonic to supersonic (in relation to the metal's shear wave velocity)—especially under high strain rates. By implementing an advanced three-dimensional discrete-continuous dislocation elastodynamics methodology, this report conducts a detailed comparative analysis against traditional dislocation dynamic approaches. It highlights the profound impact of dislocation elastodynamics on vital physical parameters, including the dynamic yield point, dislocation velocity, dislocation density, and the rate of plastic strain. This research offers valuable insights into the ultrafast mechanical behavior of metals and will play a pivotal role in the development of a dynamic constitutive metal model that comprehensively incorporates the elastodynamic effects of high-speed dislocations.

Deep and machine learning methodology in the context of application to computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A CNN-BASED APPROACH FOR OPTIMIZING LAGRANGE-GALERKIN SEARCH ALGORITHMS IN FLUID DYNAMICS

Xuan Luo[*1], Zichao Jiang[1], Bohua Huang[1], Zhuolin Wang[1], Yi Zhang[2] and Qinghe Yao[1]*

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[2]Guilin University of Electronic Technology

ABSTRACT

In this study, we introduce an innovative Lagrange-Galerkin (L-G) search algorithm, enhanced by Convolutional Neural Network (CNN) technology, to elevate the efficiency of large-scale simulations. The foundational L-G method merges a Galerkin finite element approach with a unique discretization of the material derivative, tracking fluid particle trajectories. This integration necessitates locating particles within finite elements, traditionally achieved through a step-by-step search algorithm. While effective in regular-scale simulations due to its stability and efficiency, this conventional method encounters considerable challenges in high-resolution models, particularly in handling extensive computations across densely-packed elements, thereby reducing the L-G method's iterative efficiency.

To address these limitations, the proposed method combines the L-G search algorithm with a CNN. This method leverages the CNN's capability to analyze spatial information within the finite element model and particles, extracting flow field characteristics and establishing a predictive mapping between particles and grids. Therefore, this predictive capability guides the step-by-step search algorithm towards target elements via a more direct path.

Numerical results demonstrate that the proposed method substantially reduces search costs while maintaining precision. Specifically, in the case of 3D flow simulations, the optimization rate of the proposed CNN-enhanced L-G algorithm reaches 80% compared to the classic search methods. This advancement significantly augments the L-G method's overall efficiency in large-scale simulations, offering a robust solution to the computational challenges in high-resolution flow simulation.

Computational mechanics in Canada and China: Current states of shared scientific interests and opportunities for the future cooperation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NONLINEAR ELECTROMECHANICAL TOPOLOGY OPTIMIZATION METHOD FOR STRETCHABLE ELECTRONIC INTERCONNECT STRUCTURES

Yunfeng Luo[1], Quhao Li[1], Shutian Liu[2] and YongAn Huang[3]*

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[2]*Dalian University of Technology*
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ABSTRACT

The conductive interconnect structure that connects the electrical functional devices is an important micro-nano structure in stretchable electronics. Considering that many devices rely on constant electrical currents to function, stretchable electronics would benefit from interconnects with minimal resistance variation during deformation. This paper proposes a topology optimization method for the design of stretchable interconnect structures with stable resistance under large deformation. In the proposed method, an equal material method considering geometrically nonlinear and electromechanical coupling effects is developed to evaluate the resistance of a deformed structure.

Besides, a new connectivity control method is proposed to ensure the connectivity between the inlet and outlet by making full use of the electrical problem itself. To realize the design of connected interconnect structures with minimal resistance variation during stretching, a topology optimization formulation for the design of stretchable interconnect structures is established, and the corresponding sensitivity is also analytically derived. Several numerical examples show that the proposed method is capable of computationally and intelligently generating stretchable structures with extremely small changes in resistance when stretching.

Data-driven approaches for solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DE-DEM: DISCONTINUITY-EMBEDDED DEEP ENERGY METHOD FOR SOLVING FRACTURE PROBLEMS IN SOLID MECHANICS

Zhao Luyang[*1] and Qian Shao*[1]

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ABSTRACT

Physics-Informed Neural Networks (PINN) have proven to be an effective tool for addressing forward and inverse problems of partial differential equations (PDEs). However, approximating discontinuous functions with strong nonlinearity by neural networks poses a considerable challenge, which results in high computational demands for standard PINN framework problems to solve fracture problems or multi-material problems. Besides, extra terms introduced in loss function for dealing with specific continuity requirements and internal boundaries also reduce the training efficiency. Additionally, the singular displacement and stress field in fracture problems cannot be accurately modelled in standard PINN framework.

To this end, we propose the Discontinuity-Embedded Deep Energy Method (DE-DEM). The proposed approach directly embeds the discontinuous features into the neural network by representing them with additional inputs that label specific discontinuous patterns. These additional inputs are constructed by level set functions (LSF) to flexibly represent interfaces and internal boundaries with arbitrary shapes. By controlling the properties of additional inputs, the neural network representation of physics field can be enforced to be discontinuous. This allows for the efficient solution of problems with discontinuous values or gradients at a lower computational cost. Besides, the weak form of the governing equation is utilized to train the neural network. The weak formulation intrinsically satisfies natural boundary conditions and requires lower order of gradients, augmenting the overall efficiency of the training process.

Numerical experiments are conducted on various crack patterns, including edge cracks, multiple cross cracks and interfacial cracks. Our results demonstrate the applicability of the proposed method to arbitrary crack patterns with low computational cost compared to existing PINN methods. Additionally, our approach accurately computes the singular crack tip field, enabling the straightforward computation of stress intensity factors (SIF) based on crack opening displacements. This, in turn, facilitates the prediction of the crack propagation path by combining the SIFs with suitable propagation criteria. The proposed DE-DEM framework can accurately and efficiently model the mechanical behaviors of fracture problems, which extends the application of PINN in solid mechanics.

Advanced numerical techniques for fluid flow in porous media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOWARDS EFFICIENT SIMULATION OF LARGE RESERVOIR FLOW MODELS: IMPLEMENTING AN ADAPTIVE MULTISCALE AND MULTILEVEL FINITE VOLUME TECHNIQUE FOR IMPROVED ACCURACY

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ABSTRACT

Currently, large reservoir fluid flow models may size up to a billion control volumes and sometimes the simulation of these fine-scale models is unfeasible. In general, upscaling techniques are applied to define coarser, i.e., smaller, models that can be treated by modern parallel machines at reasonable computer resources and time. This procedure naturally implies loss of information, such as small-scale fractures, vugs, and other details from the fine-scale mesh. Multiscale Finite-Volume Methods (MsFVM) have been developed to handle highly heterogeneous reservoirs using algebraic operators (restriction and prolongation) that are responsible for transferring information between the fine and coarse scales. They provide more accurate solutions than upscaled models and reduced CPU cost if compared to fine-scale simulations. Several authors have devised different strategies for obtaining accurate solutions by using multilevel or multiscale strategies. In this work, we have developed the Algebraic Dynamic Multilevel with Non-Uniform resolution (NU-ADM) using a Two Point Flux Approximation (TPFA) Finite Volume formulation for the fully implicit simulation of oil and water in highly heterogeneous petroleum reservoirs. The NU-ADM operators are based on the Algebraic Multi-Scale (AMS) operators. To better capture the physical phenomena involved, we have also developed a procedure that fits the multilevel resolution with the multilevel pressure field. This a priori procedure takes place before the pressure field calculation and is made through the fine-scale contributions to the coarse-scale transmissibility matrix coefficients. The saturation front is also adaptively captured. We have observed that the ADM outperformed the direct fine-scale solution by an order of 5. It is worth mentioning that most of these tests were conducted using the SPE10 comparative solution problem. In addition, we are using nonuniform ADM resolutions, aiming to reduce the number of active volumes of the fine-scale mesh, maintaining accuracy and improving CPU performance.

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Advanced machine learning methods for multiscale modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MECHANISTIC MACHINE LEARNING-BASED MULTISCALE MATERIAL MODELING OF METAL MATERIALS

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[1]ANSYS

ABSTRACT

Metal materials have been widely used as the most important engineering materials in automotive, aerospace, and electronics industries. Manufacturing process of metals typically induces heterogeneous microstructures across different length scales, and predicting the resulting nonlinear anisotropic behaviors by conventional single-scale empirical approaches is challenging. In this work, a data-driven multiscale modeling platform that integrates Crystal Plasticity (CP) constitutive modeling and a mechanistic machine learning method referred to as Deep Material Network (DMN) [1] is proposed. This CP-DMN framework consists of an offline training phase and an online prediction phase. The training phase for the DMN is conducted by optimizing the network fitting parameters based on the linear elastic Representative Elementary Volume (RVE) database generated using Direct Numerical Simulation (DNS) so that the accuracy of the CP-DMN is dependent on the accuracy of the RVE modeling. In the online prediction phase, the trained DMN is evaluated on a rate-dependent crystal plasticity model for predicting the complex nonlinear behaviors of RVE microstructures. Using transfer learning technique [2], a unified DMN database is created to cover a full range of grain orientations, which allows for online network interpolations for prediction of new orientations multiscale constitutive behavior. One unique feature is that the physics embedded DMN can discover the morphological features, such as grain orientation distributions hidden in RVE of metal materials. One of the industrial applications is the multiscale cold metal forging analysis. The proposed CP-DMN platform opens new possibilities in the design and concurrent multiscale metal fabrication analysis.

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Inverse and optimization problems for advanced materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NON-ITERATIVE FORMALISM FOR RELIABILITY-BASED DESIGN OPTIMIZATION VIA DECOUPLED MULTI-PROBABILITY DENSITY EVOLUTION METHOD

Meng-Ze Lyu[1], Jia-Shu Yang[2] and Jian-Bing Chen[1]*

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[2]*Xi'an University of Architecture & Technology*

ABSTRACT

Reliability-based design optimization (RBDO) is a promising methodology to address the significant challenge posed by the new generation of structural design theories centered around reliability considerations. Solving RBDO problems typically requires iterations ranging from a dozen to several hundred, with each iteration dedicated to updating the values of design variables. Furthermore, RBDO necessitates hundreds of or even more representative structural analyses at each iteration to compute the reliability measure, which serves as a foundation for determining the search direction in the subsequent iteration. This results in the double-loop problem confronted by RBDO, leading to substantial computational costs for structural reanalysis, particularly in the cases involving complex nonlinear stochastic dynamical systems. Recently, a class of non-iterative RBDO paradigms has emerged based on the newly proposed decoupled multi-probability density evolution method (M-PDEM). Specifically, the reliability is expressed as the integral of the probability density function (PDF) of the extreme response within the safety domain. The reliability of different designs can be regarded as the integral of the conditional PDF of the extreme response given the values of design variables. By leveraging the decoupled M-PDEM, a series of one-dimensional partial differential equations (PDEs) named Li-Chen equations can be solved to calculate the joint PDF of multiple responses. This enables efficient computation of the joint PDF of design variables and extreme response based on finite representative structural analyses. This method transforms RBDO into true single-loop calculations, and thereby eliminates the significant computational burden associated with structural reanalysis at different intermediate designs during the optimization iteration. Finally, the accuracy and effectiveness of this novel method are validated through several numerical examples.
Keywords: Reliability-based design optimization (RBDO); Decoupled multi-probability density evolution method (M-PDEM); Single-loop solution; Joint probability density function (PDF); Li-Chen equation.

Uncertainty quantification in structural dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ANALYTICAL SOLUTION OF GENERALIZED PROBABILITY DENSITY EVOLUTION EQUATION FOR THE ONE-DIMENSIONAL DIFFUSION PROCESS OF CHLORIDE IONS IN CONCRETE AND DIFFUSION PROCESS ANALYSIS

Xiaofei Lyu[*1] and Jie Li*[1]

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ABSTRACT

In chlorine-exposed concrete structures, chloride ion erosion leads to issues like steel corrosion and concrete damage. The diffusion-driven chloride ion transport, described by Fick's second law, involves a random diffusion coefficient due to material uncertainties. Monte Carlo Simulation (MCS) is often used to study its impact on damage like steel corrosion and concrete cracking in previous studies, but it is computationally expensive and suffers from convergence problems, compromising accuracy.
In this work, the generalized probability density evolution equation (GDEE) for the one-dimensional diffusion equation is established based on Fick's second law, and the analytical probability density function (PDF) for the diffusion concentration of chloride ions in concrete is thus derived by solving the GDEE with the characteristics method. Then the stochastic diffusion process is analyzed with the chloride ion diffusion coefficient obeying a lognormal distribution and the result shows that there is a significant spatial and temporal variability in the PDF of chloride concentration. The mean value of chloride concentration increases with time and decreases with depth, while the coefficient of variation (COV) of chloride concentration shows a tendency of first increasing and then decreasing with both time and depth. This indicates that the probability density and variability of the distribution of chloride concentration not only depend on the randomness of the diffusion coefficient, but also are closely related to the stage of the diffusion process. Meanwhile, a comparison of the numerical solution of the GDEE with the analytical PDF solution proposed in this paper reveals that when the number of subdomains increases, the accuracy of the numerical solution will increase and gradually gets close to the analytical solution, which indicates that the analytical PDF can also serve as a benchmark for measuring the accuracy of numerical methods.

Advances in multi-scale, multi-material, and multi-component Topology Optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PERFORMANCE ANALYSIS AND OPTIMISATION OF SPATIALLY-VARYING INFILL MICROSTRUCTURE WITHIN CAD GEOMETRIES USING ASYMPTOTIC ANALYSIS AND MACHINE LEARNING

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ABSTRACT

This research aims to offer an efficient digital solution to facilitate infill microstructural design within objectives generated from normal computer aided design (CAD) systems. Moreover, this approach entails a synergistic utilization of asymptotic analysis and machine learning, enabling rapid stiffness design and strength analysis of configurations filled with smoothly varying graded microstructures. The discussion is conducted in the context of an improved asymptotic-homogenisation topology optimisation (AHTO plus) framework[1]. Firstly, the key here is to deploy the microstructure and to analyse the performance of the resulting multiscale objective in the parameter domain, from which a CAD objective is mapped, usually by means of Non-Uniform Rational B-Splines (NURBS) functions. In the regularly shaped domain defined in the parameter space, another set of mapping functions are defined for the description of spatially-varying microstructure (in the parameter space), and the actual multiscale CAD objective gets represented through composition of these mapping functions with the NURBS-based functions for CAD geometry generation. When the introduced mapping functions are also NURBS-based, the proposed representation strategy becomes more favoured by CAD systems, in the sense that the CAD geometry and its infill can be tuned simultaneously but independently with a same set of NURBS basis. Moreover, our computer-aided engineering (CAE) module is also installed over the parameter domain, based on a machine-learning-based homogenisation formulation for compliance and strength analysis. Thus the finite element meshes stay unchanged although the accommodating CAD geometry keeps varying. With the aforementioned treatments, a consecutive CAD-consistent scheme is proposed. Our numerical results show that each time as the control points are moved (by a CAD designer), one may choose to wait several seconds for two-dimensional cases and/or a few minutes for three-dimensional cases, to get a CAD geometry filled with microstructure bearing optimised compliance.

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Multi-scale, multi-rate damage and fracture: Models, experiments, and simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RESEARCH ON HIGH-TEMPERATURE OXIDATION DAMAGE OF PS-PVD SPRAYED YB2SI2O7 ENVIRONMENTAL BARRIER COATINGS

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ABSTRACT

Abstract
Ceramic matrix composites (CMCs) have the characteristics of low density, high toughness, high temperature resistance, and oxidation resistance, making them the preferred material for the hot end components of next-generation aircraft engines. Environmental barrier coatings (EBCs) can effectively resist the erosion of corrosive medium such as oxygen, water vapor, and molten salts, protecting the integrity and functionality of CMCs during service. This article elucidates the microstructure and mechanical properties evolution of plasma spray-physical vapor deposition (PS-PVD) sprayed Yb2Si2O7 (YbDS) EBCs during continuous heat exposure at 1250 ℃ - 1350 ℃, develops a quantitative characterization method for isothermal oxidation damage of EBCs, and reveals the damage mechanism. The results indicate that element diffusion occurs between the top coating (TC) and bond coating (BC) layers during the oxidation process, and thermally grown oxide (TGO) is generated at the interface, which leads to an increase in nearby pores and microcracks. The TGO layer to some extent hinders the diffusion of elements, but the mismatch of thermal expansion coefficient will promote the generation of vertical and horizontal cracks in the TGO layer, which will become channels for oxygen diffusion, leading to continuous attenuation of the thickness of the BC layer. Ultimately, delamination and spalling occurred between the TGO layer and the BC layer. The oxidation kinetics curves of YbDS/Si EBCs exhibit a parabolic law. In addition, a degradation relationship was established for the mechanical properties of the BC layer. The oxidation inside the BC layer leads to an initial increase in the elastic modulus of the BC layer, which provides a pathway for internal pores and cracks caused by thermal mismatch, resulting in an irreversible decrease in the elastic modulus of the BC layer. Finally, a damage assessment method based on the fracture mechanics of the BC layer is established, providing theoretical and methodological support for predicting the lifespan of EBCs.

Keywords: Environmental barrier coatings, high-temperature oxidation, damage mechanism, microstructure evolution, mechanical properties

SIMULATION OF CRACK AND FRAGMENTATION OF MULTI-MATERIAL WITH MULTIPHYSICS

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ABSTRACT

This study explores the simulation and modeling of crack spallation and fragmentation within multi-material systems, including both ductile and brittle components. The research, detailed in our recent publications (references 1 to 3), employs hydrodynamic simulations that intricately consider multiphysics phenomena such as chemical reactions, heat transfer, phase transition, and fluid-solid interactions. Understanding the behavior of cracks and fractures in energetic materials is crucial due to its significant impact on overall performance. However, the inherent prohibitive cost of experimental studies necessitates a comprehensive reliance on simulations.

This presentation highlights advancements in 3-D simulations, co-designed with experimental data and supported by a meticulous modeling process. Detailed aspects of the modeling approach are elucidated in various recent publications, acknowledging the limitation of three references. Our contribution extends beyond simulation techniques to novel insights, fostering a comprehensive understanding of multiphysics involved in crack and fragmentation dynamics.

The synergy of simulations with experimental data offers a comprehensive perspective on the behavior of multi-materials under extreme conditions with interaction of fragmentation of ductile metal and brittle energetic material. This research not only advances fundamental understanding but also provides practical insights into the design and behavior of materials subjected to dynamic multiphysics loading.

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Modeling, optimization and computational analysis of metamaterials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATION OF SYMPLECTIC METHOD IN FORCED VIBRATION OF ACOUSTIC BLACK HOLE BEAM, PLATE AND CYLINDRICAL SHELL STRUCTURES

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ABSTRACT

In recent years, acoustic black hole structures (ABHs) have been revealed as an effective bending wave control technology. Several simulation strategies have been developed to analyze the ABH effect. However, ABH-profiled structures feature unique space-dependent wavenumber variation and wave celerity reduction over a broad frequency range. Therefore, most methods require a refined discretization scheme with high resolution in order to capture the strongly localized and highly oscillatory ABH behaviours, especially when the local wavelengths in ABH cells become shorter. Here, we introduce the symplectic method in forced vibration of acoustic black hole beam, plate and cylindrical shell structures. Various structural assemblies are provided, including: a primary beam attached by multiple ABH beams, a rectangular plate attached by multiple ABH beams, a rectangular plate attached by a ribbed or non-ribbed ABH plate, a circular cylindrical shell attached by a single ABH cylindrical shell or by periodical distributed ABH cylindrical shell. Analytical wave modes are obtained by solving the dual equations established from the vibration governing equations of each type of structural component. By considering the relationship of wave propagation, wave reflection and wave scattering, and using the developed equivalent dynamic flexibility and dynamic stiffness technique, the system equation of the structural assembly is formed in wave space. In numerical examples, forced vibration responses are calculated and validated. The significant vibration damping effect of the ABHs is verified and is explained from the point of view of waves.

Recent advances on interfaces dynamics modeling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMPROVED ACCURACY FOR REGULARIZED LINE DELTA SOURCES

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ABSTRACT

The immersed boundary method uses the Dirac delta distribution to interpolate singular forces that arise in fluid-structure interaction problems containing flexible 1D structures that are defined along moving curves. Most numerical approaches regularise the Dirac delta distribution by discretising the interface at a sequence of points and then introducing a regularisation of the Dirac delta point-source over a finite support radius of size H centered at each interface point. The corresponding delta-forcing term is then interpolated onto an underlying fluid grid (with spacing denoted h) using appropriate quadratures. We derive an analytical form for a regularised line source that can be easily implemented in an immersed boundary framework. This regularisation is constructed independently of any specific numerical method and constrained to satisfy moment properties of the Dirac delta line source distribution. The regularisation can be chosen up to a predetermined spatial order of accuracy with respect to its support H. Using both finite element and spectral approximations of a 3D elliptic test problem, we compare the results for our regularised line source to that from the usual point-delta approximation and observe that the new line-delta regularisation exhibits much smaller numerical errors. This improvement is largely due to our capturing the invariance of the line source along the direction of the immersed structure, which cannot be done for point approximations. These conclusions are supported by a careful convergence analysis in both h and H. Finally, we present some preliminary results illustrating an application of this regularised line source to 3D simulations of periodically oscillating flow through kelp forests.

A POD-BASED METHODOLOGY FOR THE DESIGN OF MODULAR CARBON-REINFORCED CONCRETE STRUCTURES

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ABSTRACT

Finite element analysis of complex structural systems, which can be put together from independent modules, is computationally expensive. To increase computational efficiency, we have developed a new model order reduction technique that exploits the idea of reducing substructures independently of each other [1]. This means that the reduction of the degrees of freedom of the global system of equations is performed at the substructure level, i.e. modules (substructures) are reduced separately before being assembled. The dominant mechanical behavior of each individual module is represented by the POD modes, which form the projection matrix. The goal is to use this method to automatically generate and evaluate a large number of possible designs for carbon reinforced structures. The prediction quality of this model order reduction technique strongly depends on the selection of the sampled data. Therefore, we introduce and investigate new sampling strategies that are more suitable for the proposed method. The proposed model order reduction method is coupled with the tied contact algorithm [2] to allow for a more flexible connection of substructures. A handful of numerical examples are shown to demonstrate the suitability of the presented methodology for the design of complex carbon reinforced concrete structures.

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Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AUTOMATED CALIBRATION OF SANISAND MODELS FOR PREDICTING SEISMIC LIQUEFACTION AND LATERAL SPREADING IN SLOPES

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ABSTRACT

The reliable prediction of liquefaction and lateral spreading in soil slopes under seismic conditions is essential for earthquake hazard mitigation and depends on the precision of advanced constitutive models. These models require meticulous calibration to authentically represent soil behavior under cyclic loading, a critical factor in seismic analysis. Traditional calibration methods for such models demand a high level of expertise and are time-consuming, limiting their practical application. Addressing this challenge, this study introduces the Automatic Parameter Calibration Tool (ACT) to simplify and accelerate the calibration of the SANISAND model, directly addressing the challenges posed by modeling soil response to seismic forces. The ACT's effectiveness was extensively validated using the comprehensive dataset from the Liquefaction Experiments and Analysis Projects (LEAP), which provided detailed characterizations of Ottawa-F65 sand under cyclic shearing. The models, once automatically calibrated based on element-level tests, were applied to simulate LEAP's centrifuge tests, examining the seismic behavior of a liquefiable slopes. Incorporating the most recent enhancements to the SANISAND model, including memory surface and semi-fluidized state features, this study demonstrates the ACT's ability to not only improve the reliability of predictions but also to make the calibration process more efficient and less dependent on specialized expertise. This progress in calibration practice broadens the accessibility of sophisticated modeling techniques to a wider audience within the geotechnical engineering community. By improving the methodology for modeling slope behavior under seismic conditions, this study makes a substantial contribution to developing more precise and user-friendly seismic risk assessment tools.

Modeling friction and wear
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SCRATCH TESTS MODELING USING FINITE ELEMENT APPLIED TO THE DESIGN OF MATERIALS' TRIBOLOGICAL PERFORMANCE

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ABSTRACT

Scratch tests can be developed on a microscale to study the tribological performance related to material phases. The investigation focused on the local effects of the second phase, which can help understand their responses when submitted to a unique abrasive action, which contributes to the design of material in tribological applications, e.g., biomedical, aerospace, and automotive. In this work, microscratch tests were conducted using a diamond cono-spherical tip of 10 um diameter against the following combination: (i) AISI 304 steel as soft homogeneous matrix; (ii) heterogeneous AISI 304 steel with TiN precipitates; (iii) AISI H13 as hard homogeneous matrix; and (iv) heterogeneous AISI H13 steel with NbC precipitates. Hard precipitates present between 6 and 10 times the matrix hardness measured using nanoindentation. During the tests, constant normal load ranges (50-150 mN: hard materials, and 40-80 mN: soft materials) were considered to assess the dominant abrasive mechanisms from the ploughing to cutting. An experimental-FEM numerical approach was implemented to obtain a robust comparison regarding the depth of penetration, friction coefficient, material removal, and specific cutting energy. The local results obtained for the hard second phases tend to allow conclusions as follows: decreased the local depth of penetration and, consequently, caused the reduction of local removed volume and increased local specific energy. When the penetration depth reached its critical size, particles were pulled out or fragmented on the material matrix, increasing the removed volume and modifying the amplitude of the specific energy. These achievements have made it possible to delineate maps to correlate abrasive micro-mechanisms on a microscale to the design of materials.

Design beyond optimization: Why, what if, and how much?
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATION-DRIVEN MULTILEVEL DESIGN OF NONLINEAR MATERIALS

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ABSTRACT

Achieving high precision, wide ranging tailorability of nonlinear structural properties has the potential to enable custom ‘designer’ materials via the construction of bulk materials from repeated, designed unit cell structures. Such designer materials could be used for improved, even optimal, application specific performance. Recent advancements have led to the emergence of multiple methods for inversely designing structures for desired nonlinear properties, including both full topology optimization inverse design approaches [1, 2] as well as reduced order model and machine learning based methods [3]. Despite the great degree of recent interest, however, there has yet to be introduced a comprehensive design approach which incorporates both the identification of the ideal target nonlinearity (for specific loading conditions) and the realization of a structure demonstrating this identified nonlinear property. Depending on the situation and objective of interest, the introduction of nonlinearity in a system can actually have a detrimental effect on the performance. Thus, it is imperative that any approach looking to improve tailored materials for impact or wave tailoring consider both a search for an ideal target nonlinearity as well as the inverse design of the constituent structure. We address this by developing a multilevel design approach, with application to dynamic response problems. The resulting collective material response and performance are compared via simulation and experiment.

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Catastrophic failure mechanics and numerical modelling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SIMULATION OF FAULT RUPTURES SUBJECTED TO FAR-FIELD LOADING AND CONSISTENT STATE OF STRESS

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ABSTRACT

The rupture of earthquake-generating faults can be considered a catastrophic event generated by frictional instability propagating along a pre-existing shear crack. Initial stress in the vicinity of a fault is a major factor influencing the nature of the rupture. The most common approach for setting the initial stress is computing the fault normal and tangential stresses according to regional stress[1]. This empirical approach is an acceptable approximation for faults with simple geometric configurations. However, for faults with complex geometries and material distributions, it is challenging to identify initial stress that is consistent with fault geometry, residual stress concentrations, far-field loading, and the heterogeneous distributions of fault strength and material properties[1,2].

In this work, we propose a method to set the initial stress distribution entirely based on mechanical considerations according to the deformation induced by far-field loading and suitable friction laws. We model the fault rupture as a propagating crack front along a pre-existing shear crack under frictional contact. As the numerical method, we use PDS-FEM due to its simple and numerically efficient treatment for modeling discontinuities[3]. The ability to set the initial stress distribution entirely based on mechanical considerations makes it possible to set the initial stress consistent with any influencing factors such as complex fault geometry, nonlinear materials, and heterogeneous frictional properties. We verified the method by reproducing the supershear rupture of a straight fault in 2D settings and the underlying Burridge-Andrew rupture mechanism. Further, we simulate the rupture of the Palu-Koro fault under different initial conditions, producing a wide range of rupture behaviors, including sub-Rayleigh and supershear ruptures.

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A MIXED HEXAHEDRAL SOLID-SHELL ELEMENT WITH SELF-EQUILIBRATED STRESSES FOR THE NONLINEAR STATIC ANALYSIS OF SHELL STRUCTURES

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ABSTRACT

Mixed finite elements with self-equilibrated assumed stresses have proven to provide several advantages for analysing shell structures [1]. They guarantee high performance when using coarse meshes and accurately represent the stress field.
This work exploits those advantages to develop a solid-shell finite element for the geometrically nonlinear static analysis of shell structures. In particular, an eight-node finite element, which has 24 displacement variables and 18 stress parameters, is developed. The displacement field is described only by translations, eliminating the need for complex finite rotation treatments in large displacement problems [2]. A Total Lagrangian formulation is used with the Green-Lagrange strain tensor and the second Piola-Kirchhoff stress tensor.
Thickness locking is cured using an assumed natural strain formulation for the transversal normal stress, and the assumed stress field eliminates shear locking. Nonlinear constitutive laws are considered using a dual decomposition approach [3]. In this way, the standard return mapping algorithms available in displacement-based formulations can be re-used for the proposed mixed finite element.
The resulting formulation is efficient and easy to implement. Computed numerical results show the accuracy and robustness of the presented element when used for both the linear and nonlinear elastic static analyses of shell structures.

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Imaging-based methods in computational medicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOWARDS A CLINICALLY RELEVANT MODEL OF THE HEART

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ABSTRACT

The majority of mechanical simulations are being performed on highly simplified models of the human heart which do not necessarily capture details relevant for implant placement and pathological analysis. High-resolution volume imaging like X-ray microtomography (microCT) can be used as a source of data for generating anatomically correct models. The main challenge in rendering it useful for modeling is controlling the variability of the models, stemming both from the specimen preparation – influence of fixation, staining, and imaging parameters, and from morphological variability, even among normal, healthy hearts. We aim to explore a pathway towards tackling the second problem by proposing a framework relying on a reduced-order model representation of the human heart with specimen variability captured by the probability distribution derived from the experimental dataset imaged with microCT. The primary representation will address normal morphology in the function of relevant metadata like age, weight, height, and estimated calcium score. The added value of metadata parameterization will also allow to postulate models with abnormalities in need of different clinical interventions.

16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Advancements in model reduction, data assimilation, and uncertainty quantification for complex physical systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GEOMETRIC DEEP LEAST-SQUARES PETROV-GALERKIN: A GRAPH AUTOENCODER-BASED REDUCED-ORDER MODEL

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ABSTRACT

The finite volume method (FVM) enjoys widespread popularity in the realms of science and engineering for its ability to conduct high-fidelity simulations of complex physical phenomena. By discretizing the integral forms of governing physical equations, FVM enables the computation of approximate solutions while preserving conservation laws. Spatial discretization of a domain is typically achieved through the use of one of two main mesh types: structured and unstructured meshes. Structured meshes employ a periodic, grid-like structure to discretize the domain. Conversely, unstructured meshes do not abide by a periodic structure, permitting mesh components to be arbitrarily ordered [1].
Deploying fine meshes for high-fidelity FVM models often incurs high computational costs that become intractable for many-query tasks, such as design optimization, uncertainty quantification, and real-time rendering. To overcome this limitation, projection-based model order reduction (PMOR) has emerged as a field of applied mathematics that aims to reduce computational cost. PMOR achieves dimensional compression by computing a low-dimensional latent space in an offline stage based on several solutions of the high-dimensional model. Then, in an online stage, PMOR projects the high-dimensional model equations onto a low-dimensional latent space, thereby reducing operational count complexity.
Recently, the deep least-squares Petrov-Galerkin (dLSPG) framework has been developed to overcome the limitations of traditional affine latent spaces when applied to advection-dominated flows [2]. dLSPG leverages an autoencoder to find a nonlinear mapping between a high-dimensional system and a low-dimensional latent space. Unfortunately, dLSPG uses an autoencoder constructed with convolutional neural networks, which are inherently dependent upon structured meshes. As a result, direct application of dLSPG to unstructured meshes is currently untenable. Fortunately, graph neural networks have been developed to extract useful information from sets of unstructured and relational data [3], making them an appropriate candidate method for generating low-dimensional latent spaces of models with unstructured meshes. We present geometric deep least-squares Petrov-Galerkin, a PMOR method that leverages a novel graph autoencoder to perform dLSPG on FVM when deploying an unstructured mesh.

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Fluid-structure interaction in interface and moving boundary problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

B-SPLINE S-VERSION OF FINITE ELEMENT METHOD FOR BOUNDARY VALUE PROBLEMS FOR FLUIDS

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ABSTRACT

Our main focus is to analyze a flapping-wing motion of a free-flying insect as a fluid–structure interaction (FSI) phenomenon. Numerical methods to deal with moving boundaries in FSI analysis can be categorized into tracking and capturing methods. However, the tracking method may generate distorted mesh for a fluid domain, which makes the calculation unstable, because the flapping motion is associated with a large deformation, movement, and contact of boundaries. On the other hand, the capturing method can not maintain high-resolution boundary layer meshes for the moving boundary layers, resulting in low accuracy.

To overcome these challenges, we use structured meshes based on the interface capturing method, and for high spatial resolution in an arbitrary local domain, we try to apply s-version of FEM (SFEM)[1], which has been studied mainly in the field of structural mechanics. Because SFEM can reasonably model an analytical domain by superimposing meshes with different spatial resolutions, it has intrinsic advantages of local high accuracy, low computation time, and simple meshing procedure. For the first step of these challenges, we have developed B-spline based SFEM (BSFEM)[2] for the Poisson equation as a simple case. Although conventional SFEM has problems with the low accuracy of numerical integration and poor convergence for solving linear equations, we have proposed BSFEM that introduces both B-spline and Lagrange basis functions and has achieved significant improvements in accuracy and convergence.

The purpose of this study is to improve localized mesh refinement in interface-capturing approaches for moving boundary problems. As the next step, we apply BSFEM to boundary value problems for fluids. In this framework, one structured mesh based on the interface capturing method is applied to the entire domain, and a higher resolution mesh based on the interface tracking method is superimposed on the boundary layers and the surrounding area which require high spatial resolution. To describe boundaries in the structured mesh, we combine immersed boundary methods with BSFEM. We verify our proposed method by solving three-dimensional flow around a circular cylinder. The results confirmed that the proposed model can obtain sufficient accurate and stable solutions.

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Physics-based data-driven modeling and uncertainty quantification in computational materials science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ML SURROGATES FOR MODEL CALIBRATION AND ERROR QUANTIFICATION IN HIGH-DIMENSIONAL PROBLEMS

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ABSTRACT

We propose a novel approach for model calibration and error quantification for high-dimensional problems with ML surrogates. In this approach, model discrepancy can be propagated from the measured quantities of interest (QoIs) to quantify uncertainty in the predictions of unmeasured QoIs. Such extrapolation situations occur when the predicted QoI is at a different location/time than the measurement of the same quantity, or when the predicted QoI is altogether different from the measured quantity. In the proposed approach, all the outputs of the system model are first mapped to an uncorrelated latent space, and surrogate models are constructed for the dominant principal features. Such mapping can readily handle high-dimensional output; in addition, for high-dimensional input, active subspace discovery is used to reduce the input dimension. Discrepancy terms are introduced in the latent space and estimated through Bayesian calibration using the measured quantities. The posterior distributions of the discrepancy terms (in the latent space) and the model parameters and observation errors (in the original space) are then propagated through the physics model to quantify the uncertainty in the prediction of the unmeasured QoIs. The formulation of discrepancy terms in the latent space offers a rigorous and efficient approach to propagate the model discrepancy information from measured to unmeasured QoIs, compared to existing approaches that either modify/augment the model parameter distributions or estimate the model form errors in the governing equations. The proposed approach is demonstrated for an additive manufacturing application, employing a heat transfer model for temperature distribution and a mechanical model for residual stress prediction in the manufactured part.

SOMA: SCALABLE OPERATOR ABSTRACTIONS FOR REPRESENTING UNSTRUCTURED MESHES

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ABSTRACT

Efficient representations of unstructured meshes play a crucial role in manipulating and navigating cell topology, a fundamental aspect of scale-resolving computational physics solver infrastructures designed for modeling complex phenomena on intricate geometries. Diverging from conventional pointer-based structures commonly found in many finite-element codes, our proposed redesign centers around incidence relation maps between entities of different types and dimensions, stored as either dense or sparse linear operators. This representation, coupled with a hash-based map for efficient entity storage and retrieval from memory, ensures portable scalability across heterogeneous architectures. This adaptability facilitates arbitrary relational queries between topological entities like up/down adjacencies and n-ring neighborhood queries to accelerate computational solvers. With support for MPI domain decomposition and a thread-safe, device-aware design, iterating through coincidence matrices stored as linear operators scalably enhances memory locality for both connectivity and adjacent queries. Additionally, the capability to define and serialize data fields on arbitrary entity types as contiguous in-memory ndarrays also provides coalesced access, especially for multicomponent systems.

In this talk, we present the details on the algorithmic infrastructure and implementation specifics of the new unstructured mesh C++ SOMA library based on a variety of backend adaptors for portably running on multinode CPU/GPU. We will also compare the computational complexity and memory footprint of our approach with some state-of-art mesh implementations, across a range of unstructured mesh query patterns that are common in solver workflows. Finally, some advanced use cases such as hierarchical mesh generation for multigrid solvers and conservative remapping for coupled multiphysics simulations which are streamlined by the algorithms developed on this infrastructure will be discussed.

Numerical modelling of composite materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTATIONAL MODELING OF UHMWPE FABRIC IMPREGNATED WITH A NEW CHEMICAL CROSSLINKER AND SHEAR THICKENING FLUID

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ABSTRACT

Ultra-High Molecular Weight Polyethylene (UHMWPE) fabrics have seen widespread utilization across various engineering domains, with a particular emphasis on impact and puncture protection. This popularity stems from their superior mechanical attributes, characterized by high strength and modulus, along with low density [1, 2]. This study presents computational modeling of a new crosslinked UHMWPE fabric infused with a Shear Thickening Fluid (STF).
To assess the impact of STF and crosslinkers on the fabric's mechanical behavior, three sample groups were prepared: untreated fabric, crosslinked fabric, and crosslinked fabric impregnated with STF. A two-layer finite element model was developed using the VFABRIC feature in Abaqus/Explicit to simulate the nonlinear in-plane and out-of-plane bending behaviors of the base fabric material. The first layer represents the material's in-plane behavior using 4-node quadrilateral membrane elements, while the shell elements in the second layer represent the bending behavior. To characterize the in-plane and out-of-plane behaviors, tensile, bias extension and Pierce bending tests were conducted, and the numerical model parameters were calibrated accordingly. Fabric elements were deemed to have failed when their stress reached a critical value in either the weft or warp yarns. Verification of the model was performed for all three sample groups under tensile and shear loading modes. Subsequently, the crosslinked UHMWPE fabric/STF model was validated using an independent puncture test. Finally, a statistical analysis was carried out to determine the effects of simulation parameters and ascertain the stress threshold for element deletion. This investigation focused specifically on the friction coefficient, identified as a crucial parameter that proved challenging to reliably obtain from physical testing.
Keywords: UHMWPE fabrics, finite element simulation, Shear thickening fluid, Puncture testing.

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Data-driven methods for modeling complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HIERARCHICAL SHRINKAGE GAUSSIAN PROCESSES: APPLICATIONS TO COMPUTER CODE EMULATION AND DYNAMICAL SYSTEM RECOVERY

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ABSTRACT

In many areas of science and engineering, computer simulations are widely used as proxies for physical experiments, which can be infeasible or unethical. Such simulations can often be computationally expensive, and an emulator can be trained to efficiently predict the desired response surface. A widely-used emulator is the Gaussian process (GP), which provides a flexible framework for efficient prediction and uncertainty quantification. Standard GPs, however, do not capture structured sparsity on the underlying response surface, which is present in many applications, particularly in the physical sciences. We thus propose a new hierarchical shrinkage GP (HierGP), which incorporates such structure via cumulative shrinkage priors within a GP framework. We show that the HierGP implicitly embeds the well-known principles of effect sparsity, heredity and hierarchy for analysis of experiments, which allows our model to identify structured sparse features from the response surface with limited data. Finally, we demonstrate the improved performance of HierGP over existing models, in a suite of numerical experiments and an application to dynamical system recovery.

CHANGE POINT DETECTION FOR INDIRECT STRUCTURAL HEALTH MONITORING

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ABSTRACT

The problem of Indirect Structural Health Monitoring or Drive-by Bridge Scanning has been extensively studied during the last decade [1]. Many of the developed frameworks suffer from the necessity for a large amount of indirect sensing data to learn and train data-driven models. Having access to such many observations may not be readily available in the context of drive-by inspection. Further, some of these techniques are based on supervised learning which makes them impractical as access to labeled data, if not impossible, is very challenging or expensive in a practical setting. In this paper, we overcome these burdens through a robust framework based on the concept of change point detection and unsupervised semantic segmentation. Time-series data are often characterized by a large degree of self-similarity due to the presence of repeated patterns. Unexpected irregularities due to any change in the state of a bridge structure introduce dissimilar patterns. Therefore, change point detection can be obtained by leveraging this self-similarity that exists in time series data. In particular, we rely on Matrix Profile, an emerging and promising tool for time series data mining, to conduct an all-pair-similarity search and discover any new patterns in time series of vehicle acceleration responses. The highest point on the matrix profile corresponds to the time series discord where a subsequence is maximally different from all other subsequences. In contrast, the lowest points on the profile correspond to the locations of the motifs with repeated patterns within the time series. Thus, by examining the matrix profile, the location of any potential anomaly can be inferred as the matrix profile at this location has its largest value due to the fact that this part is the most dissimilar part to the rest of the time series. The performance of the method is numerically evaluated through extensive investigations considering different damage cases where the effect of operational uncertainties such as road roughness, and variability in vehicle properties are taken into account. The technique is capable of working with a limited amount of data yet providing successful results which demonstrates the potential of the proposed method as a cost-effective and rigorous bridge inspection tool and opens up opportunities in the field of indirect bridge health monitoring.

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Architected materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT OF AN ON-LATTICE KINETIC MONTE CARLO MODEL FOR THIN FILM GROWTH VIA GLANCING ANGLE DEPOSITION TECHNIQUE

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ABSTRACT

The concentration of glucose in sweat has recently been measured with high sensitivity, selectivity, and reproducibility using nanostructured Ni/NiO electrodes that are manufactured through the glancing angle deposition (GLAD) technique. The GLAD technique generates nanocolumns with control over morphological properties, such as shape, porosity and film thickness, providing ample opportunities to enhance sensor performance. Currently, the selection of optimal GLAD parameters is determined experimentally through trial and error, incurring high costs in time and resources. Numerical simulations allow alternative parametric investigations of GLAD electrode geometries to obtain optimal sensor performance. In this study, surface reactions occur at the nano scale. To accurately capture these surface reactions at the nano level, our objective is to generate geometries that closely resemble the actual sensor structures to enhance the sensor modeling's predictive capabilities. To achieve this, we have utilized an on-lattice kinetic Monte Carlo (kMC) model for GLAD of Ni and NiO. Within the realm of kMC simulations, two fundamental processes occur: deposition, during which atoms settle onto the surface, and diffusion, in which atoms hop between different locations on the surface. Two crucial parameters in the deposition step, the incident angle of the incoming flux and the speed of substrate rotation are considered in the model. While the kMC method exhibits accuracy in our specific context, the process of generating a single GLAD sensor structure with a domain size of 100 nm × 100 nm × 1000 nm can be time consuming. Hence, the implementation of parallel simulation holds the potential to enhance the efficiency of the existing kMC scheme. To validate the model, the simulated structures are compared with SEM images from real cases. To the best of our knowledge, this model provides the first atomically resolved parallel model of the GLAD process. This research offers new guidance for rapidly designing highly effective sensors with increased sensitivity and lower limits of detection.

Data-driven approaches for solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING PHASE-FIELD FRACTURE USING PHYSICS-INFORMED DEEP LEARNING

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ABSTRACT

Phase-field modeling of fracture [1] recasts fracture as a variational problem which completely describes the fracture processes including crack nucleation, propagation, bifurcation, and coalescence, and obviates the need for any ad-hoc criteria. In this approach, a crack is regularized by introducing a phase-field in the formulation. Regularization leads to a nonlocal model which includes a small length scale. Resolving this length scale in computation is expensive. Hence, uncertainty quantification, material parameter identification, design optimization, among others, using this approach become prohibitively expensive. Recent advances in deep learning for applications in scientific modeling and computation [2] provide promising pathways to resolve this challenge. We explore their application to phase-field fracture modeling within the framework of physics-informed neural networks (PINNs). Since phase-field fracture is governed by a nonconvex variational energy, we employ Deep Ritz method (DRM) [3] in which the solution field is represented by a neural network (NN) and the training of the network proceeds by directly minimizing the variational energy of the system.

We solve some benchmark problems in phase-field modeling of crack nucleation, propagation, branching, and coalescence using deep learning. We first study crack nucleation in a 1-D homogeneous bar with prescribed end displacements. Using this example, we elucidate the challenges in obtaining solution using NNs with the same level of domain discretization as needed in finite element analysis. Then we discuss crack nucleation in an L-shaped panel and point to the challenges that NNs face in learning the nucleation of a crack in 2-D. We also study crack propagation and branching in a single edge notched plate under tension and shear loading. The presence of spurious energy minima makes it challenging to obtain the correct solution when prescribed displacement is not purely tensile. Finally, we show that appropriately designed NNs can learn crack coalescence as well. The details of the models and the challenges in obtaining the correct solution will be discussed.

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Continuum biomechanics of active systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOWARDS A PATIENT-SPECIFIC DECISION SUPPORT TOOL FOR STAGING OF ISCHEMIA-REPERFUSION INJURY DURING LIVER TRANSPLANTATION USING AN IN-SILICO CONTINUUM-BIOMECHANICAL FRAMEWORK

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ABSTRACT

Liver transplantation is the sole therapeutic remedy for addressing acute and chronic end-stage liver diseases. However, the increasing prevalence of elderly and multi-morbid donors and recipients introduces challenges. Grafts procured from such donors frequently manifest compromised quality due to hepatic steatosis, adversely impacting tissue structure, perfusion, metabolism, and overall organ function. The decision-making process by surgeons regarding the acceptance or rejection of marginal grafts faces a critical dilemma: The postoperative risk for the recipient has to be weighted against the risk of mortality while on the organ waiting list. Two primary challenges of marginal liver grafts involve the storage duration between organ procurement and transplantation (cold ischemia) and the ischemia-reperfusion injury (IRI).

A promising approach to unfold the intricate interplay of deformation, perfusion, and function in the liver involves computational continuum-biomechanical modeling of tissue (cf. [1]). The liver lobules, serving as the functional units, are hereby represented as a homogenized porous medium based on the theory of porous media (TPM). By incorporating cellular metabolic processes, a poroelastic multiphase and multiscale function-perfusion model is obtained (cf. [2, 3]), coupling partial differential equations on the lobular scale with ordinary differential equations on the cellular scale. Healthy liver, necrotic, and fatty liver tissue are considered as solid phases combined with a fluid phase with anisotropic perfusion. Systems biology approaches are utilized to include energy balance, death, and functionality on a cellular level. Consequently, a spatiotemporal model emerges, capable of describing the damage caused by oxygen and nutrient depletion during ischemia (cf. [3]).
The integration of experimental and clinical data for parameterization and validation alongside prior knowledge embedded in computational models significantly enhances its real-world applicability for assessing IRI based on simulating the spatiotemporal evolution of the system. A hybrid classical and machine-learning-based image analysis technique, extracts liver lobule geometry and steatosis zonation patterns from histopathological images. Laboratory data provides initial and boundary values, alongside information on the transplantation process, such as cold ischemia time. This comprehensive framework offers a predictive and patient-specific assessment of IRI, representing an important advancement towards a support tool for clinical decision-making (cf. [1]).

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A DYNAMIC WEIGHTED LOSS FUNCTION FOR ENHANCING THE PERFORMANCE OF NEURAL NETWORKS

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ABSTRACT

In machine learning process, hyper parameters are chosen in a way to decrease the prediction error and improve the convergence. However, the optimized hyper parameters have a limit in terms of enhancing the performance of the neural networks.
In this work, the datasets used for the numerical experiments arise from the resolution of partial differential equations (PDE) defined on a spatial domain. We propose a dynamic weighted loss function-based approach for neural networks that are used to learn these PDE's solutions. This a two-step process: first we train for a few numbers of epochs in a classical way then the dynamic weighted loss function replaces the classical loss function by leveraging the information from past training error histories. To validate this method, we carry out numerical experiments with different neural networks on datasets arising on three different physics: Goldstein equation [1], radiative transfer equation [2] and contact mechanics [3]. Thus, in order to demonstrate the relevance of this approach, we provide a comparison among a neural network model using a classical loss function, with and without hyper parameters optimization, and a dynamic weighted loss function for both versions.
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Emerging topology and shape optimization techniques in computational design of materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AI BASED SHAPE OPTIMIZATION OF AUTOMOTIVE RUBBER PARTS

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ABSTRACT

Rubber bumpers built into the air springs of buses perform several crucial functions, such as working together with the air spring as a secondary spring, thus modifying the original characteristics of the system when pressed together. It is a fundamental requirement that they should have a prescribed load-displacement curve. Setting this objective results in a shape optimization task. The optimization aims to achieve a specified characteristic through the geometric design of the rubber bumper while the material characteristics remain the same. In connection with the objective set, achieving the aim of the optimization will require an efficient force-displacement calculation, which is performed using the finite element method. Considering that the series of finite element runs of non-linear problems are time-consuming, therefore Support Vector Regression as a surrogate model was used to replace the costly engineering simulations and to support the shape optimization. A simulated annealing algorithm with an adaptive search space and different cooling schedules was developed for the shape optimization of rubber bumper. The novel method is capable to solve the optimization task of the rubber bumper with high accuracy in plannable time and high automation. Due to the automated process, the developed method can be integrated into product development.

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DISCOVERING INTERPRETABLE PHYSICAL MODELS USING SYMBOLIC REGRESSION AND DISCRETE EXTERIOR CALCULUS

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ABSTRACT

Mathematical modeling and numerical simulations are powerful tools for understanding physical systems within contemporary scientific research and engineering. The abundance of data has enabled the use of Machine Learning (ML) to enhance model identification from experiments and improve the accuracy and performance of the simulations. However, purely data-driven models often suffer from limited generalization and interpretability. To address these challenges, Symbolic Regression (SR) has been proposed to discover equation-based models, which are inherently interpretable and amenable to analysis. Previous investigations have been limited to classical equations of Physics and mainly to single-Degree-Of-Freedom or dynamical systems, which are governed by algebraic or ordinary differential equations. In this work [1], we advance the state-of-the-art by combining SR with Discrete Exterior Calculus (DEC) [2] to enable the discovery of field theories. The use of a universal, discrete mathematical framework specifically tailored for physics enhances the generalizability of the recovered models, even in small-data scenarios. Additionally, DEC allows to implement strongly-typed SR, thus ensuring the mathematical and physical consistency of the recovered model equations and reducing the search space of the SR. We validate our approach by successfully re-deriving three Continuum Physics models from synthetic experimental data: the Poisson equation, Euler's Elastica, and the Linear Elasticity equations. Finally, we present preliminary results regarding the use of our framework to derive coarse-grained models of crack propagation in soft polymers, a research problem that aims at elucidating the fundamental damage and fracture mechanisms in these materials, which are still poorly understood.

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Virtual elements for partial differential equations on polytopal meshes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A C 1 CONFORMING ARBITRARY-ORDER TWO-DIMENSIONAL VIRTUAL ELEMENT METHOD FOR THE FOURTH-ORDER PHASE-FIELD EQUATION

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ABSTRACT

We present a conforming virtual element method [1] for the two-dimensional High-Order Phase Field (HOPF) equation [2]. This is a fourth-order equation, and our numerical approximation relies on the design of an arbitrary order accurate, virtual element space with C 1 global regularity. Such regularity is guaranteed by taking the values of the virtual element functions and their full gradient at the mesh vertices as degrees of freedom. High-order accuracy also requires edge polynomial moments of the trace of the virtual element functions and their normal derivatives. A set of representative test cases assess the behavior of the method.

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Advances in neural operators for scientific modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEEPONETS FOR FORWARD AND INVERSE PROBLEMS IN ASTROPHYSICAL FLUID DYNAMICS

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ABSTRACT

Machine learning has seen widespread application in fluid mechanics. Traditional neural networks, which approximate functions by mapping inputs (either scalar or fields) to outputs, are not well-suited for learning parametric systems. These systems typically involve inputs that include both parameters and coordinates, and their outputs are solutions. To address this, Deep Operator Networks (DeepONets) have been developed.

We present two papers focusing on the application of DeepONets in astrophysical fluid dynamics governed by the Navier-Stokes equations. The first paper introduces a ML tool based on DeepONets mapping PDE parameters to their corresponding solutions. This tool is trained using simulation data. We observed that vanilla DeepONets struggle to accurately represent sharp spatial features in solutions, which vary with input parameters. This indicates a difficulty in learning the nonlinear relationship between PDE parameters and coordinates. To overcome this, we propose a modified DeepONet architecture that converges faster and reduces the error in sharp features by an order of magnitude. Our tool can predict solutions at a rate of one per second on a CPU and forty per second on an NVIDIA V100 GPU, significantly faster than traditional numerical methods, which require thousands of CPU hours. We extensively tested the prediction accuracy of our tool and demonstrated its application in astronomical problems.

The second paper addresses the inverse problem: inferring parameters from unseen solution data. We combine trained DeepONets with a state-of-the-art optimization algorithm, the Covariance Matrix Adaptation Evolution Strategy (CMA-ES). This combination employs an iterative forward-backward approach. In each iteration, we update the PDE parameter samples to converge towards ground truth values, generate new parameter samples, evaluate the corresponding solutions using DeepONets, and compare them with the data to be fitted. The fitness of parameter candidates to the data is assessed by CMA-ES, which then updates the PDE parameter samples for the next iteration.

We tested our inverse problem solver on a group of datasets, each containing 256 solutions. Running on an NVIDIA GPU, this tool can evaluate 50,000 parameter candidates in thirty minutes and iterate the parameter samples a hundred times. Due to this extensive exploration of the parameter space, our method infers parameters with an error within 1% of the ground truth. It also remains robust with noisy or obscured data (data with missing pixel values), maintaining the same level of accuracy as with clear data. We demonstrate the potential application of our tool in astrophysical fluid dynamics.

Phase-field interface modeling for multiphase and multiphysics simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A 3D PHASE-FIELD BASED EULERIAN VARIATIONAL FRAMEWORK FOR MULTIPHASE FSI WITH CONTACT BETWEEN SOLIDS

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ABSTRACT

Using a fixed Eulerian mesh, interface-capturing approaches such as volume-of-fluid, level-set and phase-field methods have been successfully utilized for a broad range of moving boundary problems involving multiphase fluids and single-phase fluid-structure interaction. Nevertheless, multiphase fluids interacting with multiple solids are rarely explored, especially for large-scale finite element simulations. In this work, we introduce a novel parallelized three-dimensional fully Eulerian variational framework for simulating multiphase fluids interacting with multiple deformable solids with contact between solids. In the framework, each solid or fluid phase is identified by a standalone phase indicator. Moreover the phase indicators are initialized by the grid cell method, which restricts the calculation to several grid cells instead of the entire domain and thus evolved by the corresponding phase-field equation in the fixed mesh. A diffuse interface description is employed for a smooth interpolation of the physical properties across the phases, yielding unified mass and momentum conservation equations for the dynamics. For each solid object, temporal integration is carried out to track the strain evolution in an Eulerian frame of reference. The coupled differential equations are solved in a partitioned manner and integrated via nonlinear iterations. We first verify the framework against reference numerical data in a two-dimensional case of a rotational disk driven by lid-cavity flow. The case is generalized to a rotational sphere driven by lid-cavity flow to showcase large deformation and rotational motion of solids and examine the convergence in three dimensions. We then simulate the falling of an immersed solid sphere on a solid block under gravitational force to demonstrate translational motion and contact of solids in a fluid environment. Finally, we demonstrate the capability of our proposed framework for a ship-ice interaction problem involving multiphase fluids with an air-water interface and contact between a floating ship and ice floes.

Recent advances in computational fracture mechanics and failure analysis
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ON ELASTIC ANISOTROPY OF 3D PRINTED ACRYLONITRILE BUTADIENE STYRENE

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ABSTRACT

Additive manufacturing (AM) allows for part fabrications by successive layer deposition with advantages like flexibility in design and material waste reduction [1]. Within the AM technologies, fused filament modeling (FDM) is one of the most widespread processes because of its low-cost implementation and accessibility [2]. However, empirical models are not adapted for the description of the behavior of AM parts. One of the challenges is to develop appropriate models for the prediction of AM material responses considering the range of process parameters. In this study, integrated digital image correlation (I-DIC) [3] is used for the identification of constitutive parameters of two configurations of acrylonitrile butadiene styrene (ABS) samples.
Two single edge notched tension (SENT) samples obtained by FDM have been tested. In one sample, the filaments were oriented at ±45° and in the other one they followed the direction of maximum strains. During the tests, the images of both sample surfaces were recorded. The acquired images were used for the calibration of constitutive parameters via I-DIC. Before launching the identification step, some pre-processing was made. The DIC results were used to determine the standard displacement and force uncertainties. Several computations using coarse meshes to approximate the solution at convergence, estimating the identifiability of the material parameters and checking whether the investigated solution corresponded to a local or global minimum were conducted. After this preliminary step, complete computations were run with fine meshes. The uncertainties associated with each calibrated parameter were estimated using their covariance matrix, and the evaluation of their identifiability using the total Hessian matrices at convergence were possible.
The calibrated parameters were used to conduct simulations of simple tensile tests. They were compared to stress-strain curves obtained in others studies on standard tensile tests. It is shown that an isotropic elastoplastic model calibrated from one SENT specimen described correctly the behavior of 3D printed ABS parts independently of the internal infill strategy.

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DG0/CR DISCRETIZATION OF PHASE-FIELD FOR FRACTURE

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ABSTRACT

Phase-field methods for fracture have shown their great abilities over the last 20 years at computing crack paths in elastic domains. However, due to the Ambrosio-Tortorelli regularization of the elastic energy, one necessarily has $\sigma \cdot n = 0$ in the crack. This forbids the direct imposition of a pressure p inside the crack as $-pn \neq 0 = \sigma \cdot n$.

To remedy this problem, we propose a new discretization of the Francfort-Marigo functional which does not consist in using P^1 Lagrange elements and an Ambrosio-tortorelli regularization.
Building on the previous work [Bourdin and Marazzato, 2023], we use instead Discontinuous Galerkin (DG) and Crouzeix-Raviart (CR) mixed elements. The phase-field term is conserved in its usual form but the coupling between elasticity and phase-field happens in a penalty term and not through the elastic term. This allows to impose $\sigma \cdot n = -p n$ inside the crack.

We propose to explain why this new methodology is coherent with the Francfort-Marigo functional though Γ-convergence and show its relevance though numerical examples.

Multi-scale, multi-rate damage and fracture: Models, experiments, and simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPERIMENTAL INVESTIGATION AND MODELLING OF DAMAGE PHENOMENA IN FDM-3D PRINTED MATERIALS

Sonia Marfia[*1], Denis Linardi[1] and Elisabetta Monaldo[1]*

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ABSTRACT

In the last decade, the additive manufacturing based on fused deposition modelling (FDM) has become increasingly attractive in diverse engineering fields. For successful applications of 3D printed structural elements as end-user parts, reliable performance in terms of stiffness and strength properties has to be ensured. There are numerous experimental studies that mainly investigate the stiffness properties of the 3D printed materials as a function of several printing parameters. However, only few studies, have characterized the failure mechanisms of 3D printed samples and the crucial role of the bond properties between adjacent fibers on the overall strength of printed elements [1].

This work aims to propose a deep experimental campaign in order to investigate the damage phenomena in 3D printed materials as a function of printing parameters. On the base of these experimental results, an innovative non-local orthotropic damage and plasticity phenomenological model is proposed. The effective mechanical behaviour of 3D printed structural elements is described by means of the composite laminate theory {2]. Each layer of the laminate is described with an orthotropic elasto-plastic constitutive behaviour and the Tsai-Hill yield limit function is adopted. Moreover, the stiffness degradation of the material is described by means of three damage variables specially introduced to describe the different damage phenomena (i.e., fiber failure, inter-layer and intra-layer damage) occurring under different loading conditions, as highlighted by the analysis of the 3D printed samples after the failure.

Some numerical applications are carried out, comparing numerical results with the experimental ones. The proposed model proved to be able to reproduce the range of failure modes from brittle-like to ductile that characterize the mechanical behaviour of 3D printed materials.

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Data-driven methods for modeling complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODEL IDENTIFICATION: A HYBRID SINDY-NONLINEAR KALMAN FILTERING APPROACH

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ABSTRACT

A new data-driven procedure for model identification in structural dynamics is proposed. The method features a combination of SINDy (Sparse Identification of Non-linear Dynamics) for model discovery and nonlinear Kalman filtering for data assimilation. To properly deal with problem nonlinearities, solutions based on the extended or the unscented Kalman filter are offered, in the latter case avoiding to handle the Jacobian of system evolution and leveraging parallel computing. SINDy is based on the solution of a sparse regression problem starting from time-series data [1]; Kalman filters can then be exploited to set the coefficients weighting a dictionary of pre-defined functions, that collectively mimic the actual system dynamics. Within a joint identification framework, the input to the data assimilation problem can be represented by system dynamics (like nodal displacements, velocities, and accelerations in a space-discretized model), forcing terms and, possibly, additional parameters describing some physical properties of the system itself (like e.g. its stiffness and damping). Aiming to provide an adaptive digital twin of mechanical systems, the aforementioned parameters may evolve in time due to degradation phenomena. To avoid performing SINDy anytime the output of the digital twin is characterized by a too-large drift away from the measured response, and to also account for prior information regarding the identified system, the use of nonlinear filters is here explored, see e.g. [2]. The offered solution has clear computational advantages to move towards real-time monitoring strategies of existing structures: by modifying on-the-fly the values of the physical parameters used as input for the SINDy functions, the methodology can also overcome issues related to the inadequacy of the modeling assumptions [3]. The methodology is assessed against some case studies characterized by either a linear or a nonlinear behavior, to testify the improvement over other state-of-the-art techniques.

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Current trends in phase-field modeling and computations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ENERGY-CONSISTENT SPLITS IN PHASE-FIELD MODELLING OF ANISOTROPIC BRITTLE FRACTURE VIA PHYSICALLY INTERPRETABLE STRAIN MODES

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ABSTRACT

In the realm of phase field models for brittle fracture, a pivotal consideration involves the division of strain energy density functions into damaging and non-damaging components.

In contrast to isotropic materials, strategies for decomposing the strain-energy density of anisotropic materials represent ongoing research challenges. Existing solutions often prove inconsistent, either from an energetic or a constitutive perspective. Consistent generalizations of strain-energy decompositions in anisotropic materials are limited [1]. One approach employs principal value decomposition, allowing for the introduction of either a generalized version of spectral energy decomposition or an orthogonal decomposition of the strain tensor using the scheme proposed by He and Shao [2]. Another approach is founded on a generalized version of the hydrostatic and deviatoric split in terms of energies.

Analytical formulas are notably absent in all cases, owing to the spectral decompositions of energy-related expressions or the stiffness tensor. Additionally, unlike isotropic materials, the proposed decompositions suffer from a weak kinematic interpretation, impacting the physical interpretability of results. Furthermore, existing approaches often exhibit weaknesses in terms of numerical robustness.

This study introduces a novel approach for transversely isotropic materials, providing easily applicable analytical formulas and a succinct physical interpretation. The method builds upon recent findings by Marino and Wriggers [3], utilizing Walpole's formalism for representing transversely isotropic stiffness tensors. Leveraging this framework, the study achieves an energy-consistent split, grounded in kinematic arguments, of strain energies for transversely isotropic materials. This innovative approach is detailed within the context of the phase-field method for brittle damage of transversely isotropic materials, with its effectiveness explored through numerous numerical examples.

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Multi-scale, multi-rate damage and fracture: Models, experiments, and simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A METHODOLOGY TO QUANTIFY ENTROPY GENERATED DURING FATIGUE OF CF/PEKK COMPOSITE LAMINATES: CONSTITUTIVE MODEL

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ABSTRACT

Fatigue failure of composite materials results from the accumulated effects of irreversible phenomena such as damage propagation and plasticity. Based on the Clausius-Duhem inequality representation of the second law of thermodynamics, any dissipative phenomenon generates entropy. Therefore, the concept of entropy generation yields a natural theoretical candidate to predict the fatigue lifetime of these materials. In fact, previous research has proven the total entropy generated during fatigue of composite materials to be constant, independently of stress ratio, loading frequency or stacking sequence, thus demonstrating promising capabilities as an alternative fatigue failure criterion. However, materials selected for experimental validation have solely consisted of thermoset-based composites. With the growing application in thermoplastic composites for aerospace structural components comes the interest to extend and validate the entropy generation concept to these materials. Given the rate- and temperature-dependent behavior of thermoplastics, the dissipation inequality formulation must account for dissipative phenomena such as plasticity, viscosity, and friction in the material constitutive laws. This work proposes a reformulation of the dissipation inequality using a continuum damage-based model at the laminate level that accounts for viscous, thermal, and plastic effects. Material properties included in the proposed constitutive model have been calibrated with experimental testing of carbon fiber/PEKK composite samples. Using the proposed form for the dissipation inequality, a second part of this work will quantify the entropy generated during stress-controlled tension-tension fatigue of carbon fiber/PEKK composite samples with two stacking sequences at different loading frequencies and maximum stress levels.

Theory and application of provably-robust and efficient high-order methods for high-fidelity computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A HYBRID SHOCK FITTING-CAPTURING METHOD FOR HIGH-SPEED FLOWS

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ABSTRACT

High-Order Implicit Shock Tracking (HOIST) is a class of methods that computes the solution of a conservation law and the nodal coordinates of the shock aligned mesh through the formulation of a PDE-constrained optimization problem. The PDE constraint uses a DG discretization with conservation, stability and high-order accuracy properties. A sequential quadratic programming method is used to converge simultaneously the DG solution and the nodal coordinates, which avoids nonlinear stability issues due to a non-aligned mesh. The method allows high-order approximations of high speed flows without requiring extensive mesh refinement in non-smooth regions. Curved interfaces are tracked to high-order accuracy by the use of high-order elements to generate curved elements.

This work presents a new methodology that integrates shock capturing and shock tracking to leverage the advantages of each. Strong bow shocks will be fully tracked because they play a critical role in the prediction of aerodynamic forces and can be readily fit with the grid using modern shock tracking techniques. Weaker secondary shocks that have proven more difficult (and less critical) to fit will be captured using artificial viscosity.

MODELLING OF SEISMIC WAVES USING A DECOUPLED DISCRETE-TIME GRID-WAVE PROPAGATION MODEL

Andrea Marti[1], Carlos E. Ventura[1] and José R. Martí[1]*

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ABSTRACT

The development of an Urban Real-Time Earthquake Early Warning system is being undertaken at the University of British Columbia. This system is based on having a coordinated dense network of low-cost seismic stations spaced 50-100 m apart in a grid formation. This grid formation allows us to achieve a very high spatial and temporal resolution within a city. It can capture seismic wave frequencies up to 20 Hz under high variability in soil conditions, which can change within as little as 1 km. The seismic stations are mounted to a building, house, bridge, substation, or other infrastructure. Each station comprises a MEMS tri-axial accelerometer, a Raspberry Pi processing board, and a 5G cellular transmitter. Associated with this physical hardware is a discrete-time wave propagation model between any two nodes of the grid, where every node in the wave model corresponds to the physical geographical coordinates of the seismic stations. As the data arrives at each physical node, the grid wave propagation model computes the predicted full shape of the strong S-wave and the other waves before they arrive at the infrastructure.

The grid-wave propagation model is an extension of the electromagnetic transients numerical solution method (EMTP), well-established in the field of electromagnetic wave transients in electric power systems. The EMTP-wave model is based on separating the 2nd-order wave equation into two 1st-order PDEs. This separation decouples each line between the connected nodes into two decoupled segments. Each segment contains a parameter called the characteristic impedance, representing the characteristic of the medium the wave propagates through, and a parameter representing the losses from wave attenuation. This decoupling makes the [Y] matrix in the grid solution [Y][A]=[B] to be fully diagonal making the solution to be of order N, where N is the number of nodes.

This decoupling is significant since it reduces the order of the solution from N^2 without decoupling using sparsity to only N for each point of the wave. For example, a 10km x 10km grid spaced 100 m apart (10,000 nodes) can be solved in approximately 80 milliseconds on a 3.7 GHz computer, while it would take 13 min for the non-EMTP solution. In addition, because each line segment contains the localized soil parameters, the strength of the wave is automatically accounted for when solving the system of nodal equations, allowing for a more accurate description of the wave magnitude before it reaches the Critical Infrastructure.

Mathematical modeling and simulation for social, environmental, and disaster prevention issues
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELLING AND SIMULATION OF THE DYNAMIC RESILIENCE OF COMPLEX SYSTEMS DURING LARGE DISASTERS USING THE I2SIM FRAMEWORK

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ABSTRACT

i2SIM is a non-linear system optimizer and software package that models the interdependencies among a city's critical infrastructures and maximizes the allocation of resources towards a global objective function accounting for each infrastructure's physical constraints. Multiple heterogeneous physical and social infrastructures are affected after a disaster, such as electric power substations, water stations, gas pipes, communication networks, transportation routes, hospitals, emergency responders, and the community's economy, social cohesion, and livelihood.

In i2SIM, each infrastructure is considered a functional block (Cell) where the Cell's transfer function is defined by a relationships table called a Human Readable Table (HRT). The functional relationship for each Cell is given by the function: y(Cell)=min{f_1(input_1), f_2(input_2),..., f_n(input_n)}, where y(Cell) is the output of the Cell, and f_i is the functional relationship between input_i and the Cell's output, assuming all other inputs are available. For each input function, the HRT is constrained to an upper limit (infrastructure capacity) and lower limit (usually zero). These relationships define a closed-loop mathematical system of non-linear equations with limits. This closed-loop formulation allows a) the identification of the weakest (limiting) inputs to each system, b) the sensitivity of the output of each system on each one of its inputs, and c) the use of optimization techniques to find the minimum allocation of resources in each Cell that will result in the combined system of infrastructures objective function, such as community wellbeing.

During a disaster, when multiple systems fail simultaneously, the reliability of each system is a function of its level of operation and the level of operation of the other systems that it depends on. However, each individual infrastructure (e.g., the power grid) is unfamiliar with the internal details of the other infrastructures that it depends on (e.g., the water system, the health system). i2SIM calculates the functional and data requirements shared among infrastructures and communicates this information to all interdependent infrastructures. This coordination allows a global reliability measure to be defined and acted upon during the response without each infrastructure requiring full knowledge of the others' internal workings. One current use of i2SIM is for real-time consequence analysis when simultaneous wildfires occur, and decisions on which fire to extinguish first must be made. The consequences of a disaster depend on both pre-disaster measures for robustness and post-disaster coordinated response actions, and this pre-disaster-post-disaster timeline using i2SIM defines dynamic resilience indices for the total cost (monetary and social) of a disaster.

Novel mathematical and numerical models for multiphysics and multiscale systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FINITE ELEMENT INTERPOLATED NEURAL NETWORKS FOR SOLVING FORWARD AND INVERSE PROBLEMS

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ABSTRACT

We propose a general framework for solving multi-scale forward and inverse problems constrained by partial differential equations (PDEs), where we interpolate multi-layer feed-forward neural networks onto conforming finite element spaces to represent the unknown model state variables (for forward and inverse problems), and the (partially) unknown data (only for inverse problems) [1]. This approach is coined with the term FEINNs. For forward problems, an approximate solution is obtained by designing a robust, well-posed PDE residual loss functional, which is then minimized using gradient-based optimization techniques. In the case of inverse problems, and additional term that measures the data misfit among (partial and potentially noisy) observations of the model state variables and the current model is also included in the loss function, and we propose an adjoint-free effective one-loop solver with an initial data fitting step to obtain a cheap initialisation of the neural network. The framework overcomes the challenges related to the imposition of boundary conditions and the choice of collocation points in physics-informed neural networks, as well as those related to the cell and facet integration of variational physics-informed neural networks. Besides, the framework is suitable to tackle multi-physics and multi-scale problems (e.g., problems with singularities and/or shocks) when combined with octree-based multi-resolution meshes and a-posteriori error estimators. A comprehensive numerical experiment set confirms the framework's capability of handling several forward and inverse problems, including some posed on complex geometries. While the experiments reported will be restricted to problems discretized using grad-conforming finite element spaces, the framework can be generalized to problems discretized using div- and curl-conforming spaces, such as, e.g., flow in porous media or the Maxwell equations. Remarkably, among other striking findings, the trained neural networks can be orders of magnitude more accurate than the finite element solution on the same mesh for smooth problems, even for those in which the solution has an internal shock, thus confirming the ability of the framework to unleash to a large extent the non-linear, built-in adaptive, approximability properties of neural networks. Besides, unlike adjoint-based inverse PDE solvers with finite element spaces to represent all unknowns, all the inverse problems tackled in the study with FEINNs could be flawlessly solved without the need of a regularization term in the loss functional.

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Advanced analysis of steel and steel-concrete composite structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SEISMIC ANALYSIS AND RETROFITTING SOLUTIONS FOR A PILE-SUPPORTED SHIPLOADING INFRASTRUCTURES

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ABSTRACT

This paper provides a comprehensive exploration of seismic analysis and retrofitting solutions tailored to pile-supported shiploading infrastructures, with a specific focus on a Class D site near Vancouver. A critical assessment of ASCE 61-14, a key standard in marine seismic design, is conducted, integrating insights from observed marine facility behaviors during seismic events and tracing the evolution of seismic design provisions from historical practices to contemporary standards.

In the assessment phase, nonlinear static analysis is employed, emphasizing a high-fidelity finite element method. Our analysis centers on a specific case study, a pile-supported wharf near Vancouver, delving into damage localization in both superstructure and soil below the mud line. This illuminates the potential of advanced modeling techniques to enhance earthquake-resistant design in pile-supported structures.

Furthermore, the paper explores the consequences of relying on simplified seismic design analyses, particularly examining diverse impacts of earthquake ground motions. Through nonlinear dynamic analysis, the work unveils nuances associated with different seismic design strategies, highlighting the importance of dynamic analysis in fortifying earthquake-resistant design for such structures.

Principal contributions to the field include a nuanced understanding of seismic design requirements, advanced modeling techniques for damage localization, and insights into the implications of seismic design choices. By addressing these aspects, the paper contributes valuable insights and practical recommendations for enhancing earthquake-resistant design in marine facilities, particularly those with pile-supported shiploading infrastructures.

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Multiphysics and data-driven modeling for cardiovascular biomedicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NEURAL NETWORK BASED SURROGATE MODELING OF CARDIAC FUNCTION ENCODING GEOMETRIC VARIABILITY

Elena Martinez[*1], Matteo Salvador[1], Fanwei Kong[1], Beatrice Moscoloni[2], Mathias Peirlinck[2] and Alison Marsden[1]*

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ABSTRACT

The combination of physics-based modeling with data-driven methods enables the clinical translation of computational cardiology. Today, the use of rigorous differential equations combined with machine learning tools allows patient-specific parameter personalization with uncertainty quantification in time frames compatible with clinical practice. However, accurate and efficient surrogate models of cardiac function are still mostly geometry-specific and require retraining for different patients and pathological conditions. We propose a novel computational framework to embed different cardiac anatomies into neural network based surrogate models. We generate a dataset of numerical simulations using mathematical models based on differential equations. We consider Branched Latent Neural Maps (BLNMs) as an accurate and efficient computational tool to encode complex space-time fields into a neural network. We employ statistical shape modeling and deep learning methods using signed distance fields to represent different human hearts. This framework would allow for fast and robust parameter estimation on patient cohorts without the need to modify the surrogate model.

Physical models and reduced order models augmentation with data for physics-informed machine learning in real-world applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GRAPH NEURAL NETWORKS FOR GEOMETRIC DESIGN OF STRUCTURES IN PLASTIC REGIME

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ABSTRACT

This research is dedicated to advancing data-driven modeling of plasticity, with a distinctive emphasis on achieving speed-ups rather than developing constitutive models, which are already known to us. Our primary goal is to provide analysts with an efficient tool for designing and analyzing structures undergoing plastic strain within strict real-time constraints

Leveraging Graph Neural Networks (GNNs) and synthetic data generated from Finite Element Method (FEM) simulations, our approach showcases robust generalization capabilities. The motivation behind this work lies in the imperative need to reduce computational costs, a critical objective compared to the prevalent reliance on Finite Element Method (FEM) approaches. By incorporating prior knowledge through data-driven approaches, our research significantly accelerates predictions, potentially revolutionizing the process design for working with plastic materials.

Various parameters, including specimen height and length, underwent tuning to delineate diverse geometries. The model was then tested on unforeseen geometries, illustrating its robustness and generalization capabilities in both interpolation and extrapolation scenarios. This study contributes to the conference by introducing an innovative approach to plasticity modeling, with a focus on efficiency, generalization, and cost reduction in structural analysis. It marks a stride forward into novel and accelerated tools for the design of structures in the plastic regime, promising advancements in the field of real-time analysis.

Current trends in phase-field modeling and computations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHASE FIELD MODELLING OF FATIGUE CRACK GROWTH: OPPORTUNITIES, ACCELERATION SCHEMES AND COUPLED PROBLEMS

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ABSTRACT

Predicting fatigue failures remains one of the most elusive challenges for scientists and engineers. In this work, we develop a comprehensive phase field model capable of predicting fatigue failures of arbitrary complexity. Through comparison with experiments, the model is shown to accurately predict the fatigue behaviour of materials, including S-N curves, Paris law crack growth, the influence of the load ratio, mean stress effects, stress concentrator factors and the endurance limit. In brittle and quasi-brittle solids, the model is able to predict fatigue crack growth rates from S-N curves, and vice-versa. Moreover, the framework is extended to account for the presence of hydrogen, which is known to significantly impact the fatigue resistance of metals. The resulting coupled deformation-diffusion-damage model is shown to be able to qualitatively and quantitatively capture the role of hydrogen in increasing fatigue crack growth rates and decreasing the number of cycles to failure. Our numerical experiments enable mapping the three loading frequency regimes and naturally recover Paris law behaviour for various hydrogen concentrations. In addition, Virtual S–N curves are obtained for both notched and smooth samples, exhibiting a good agreement with experiments. Aspects of the numerical implementation will also be discussed, showing how complex fatigue cracking phenomena in 2D and 3D can be captured, over millions of cycles, through the development and use of new acceleration schemes.

Advances in neural operators for scientific modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COUPLING VARIATIONAL DATA ASSIMILATION AND OPERATOR LEARNING FOR EFFECTIVE STATE ESTIMATION ON COMPLEX SYSTEMS

Stiven Briand God Massala Moussounda[1], Ludovic Chamoin[2] and Massimo Pica Ciamarra[3]*

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ABSTRACT

We introduce a hybrid twin approach to solve physical systems modeled by parametrized Partial Differential Equations (PDE). Our approach, combines the variational data assimlation(PBDW) [1] with operator learning(Deeponets)[2] to reconstruct the state of an imperfect physical system given many observations. The PBDW method is a non-intrusive, reduced basis, in-situ data assimilation framework, that estimates the solution of a biased model given many observations. This method provide a state estimate framework for parameterized model that estimate both the anticipated and the non anticipated physics while ensuring orthogonality between both parts. The anticipated physics is approximated by a background space constructed with reduced basis while the non-anticipated physics is infered by a Deeponets. The hybrid twin was performed using two approaches to ensure orthogonality. A first approach with a weak constrain, that regularizes the loss function of the neural operator with the dot product between the un-anticipated physics and the background space, in this case the trunk net learn from the whole space but the constrain is only garanteed in the training stage. And a second approach with strong constrain where the trunk is replaced by a set of basis function, each orthogonal to the background space by construction, that garantee orthogonaly in both the training and inference stage of the un-anticipated physics. The hybrid twin was applied on a 2D Helmoltz equation on a homogeneous and bounded domain with a biased source, to showcase its potential for solving complex physical systems.

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operators

Numerical methods, mathematical modeling and analysis in material science
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MOMENTUM SPACE METHOD FOR ELECTRONICS OF MECHANICALLY RELAXED INCOMMENSURATE 2D MATERIALS

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ABSTRACT

Since their discovery by Geim, 2D materials have become a hotbed of research due to their novel structure. Layering materials with tunable relative twists allows for a vast range of possible materials and corresponding electronic and mechanical properties. However, this stacking typically leads to an aperiodic, or incommensurate, material due to lattice mismatch or rotational misalignment. When two materials vary only by a small twist, as is the case for magic angle physics, large moire patterns arise and mechanical relaxation effects have significant impact on electronic structure.

In this work, we discuss configuration and momentum space methodologies to build algorithms for computing electronic observables including quasi-band structure for incommensurate bilayers for ab-initio single-particle tight-binding models. Mechanical relaxation effects are modeled via a continuum model, and are incorporated into the electronic tight-binding model. These models allow for prediction of electron transport properties, and provide a platform for construction of many-body models describing unconventional superconductivity and other many-body effects at magic angles. We exploit the ergodicity of the misalignment, and for appropriate materials (such as those with conic or parabolic bands) we use carefully selected perturbative expansions in momentum space with a thorough error analysis to describe the effects of the large moire scale.

SciML in the real world
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICS-CONSTRAINED DATA-DRIVEN VARIATIONAL METHOD FOR DISCREPANCY MODELING

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ABSTRACT

The effective inclusion of a-priori knowledge when embedding data in physics-based models of dynamical systems can ensure that the reconstructed model respects physical principles, while simultaneously improving the accuracy of the solution in the previously unseen regions of state space. This talk presents a physics-constrained data-driven discrepancy modeling method that variationally embeds measured data in the modeling framework. The hierarchical structure of the method yields fine scale variational equations that facilitate the derivation of residuals which are comprised of the first-principles theory and sensor-based measurements of the dynamical system. The embedding of the sensor data via residual terms leads to discrepancy-informed closure models, thereby resulting in a method which is driven not only by boundary and initial conditions, but also by measurements that are taken at only a few observation points in the target system. Specifically, the data-embedding term behaves like a residual-based least-squares loss function, thus retaining variational consistency. The structure of the loss function is analyzed in the context of variational correction to the modeled response wherein loss function penalizes the difference in the modeled response from the measured data that represents the local behavior of the system. Formulation is then extended for transient analysis and the effect of the variationally embedded loss function on time dependent response of the system is analyzed under a variety of loading conditions. Specifically, the damped solution and correct energy time histories are recovered by including known data in the undamped situation. The enhanced stability and accuracy of the DDV method is manifested via reconstructed displacement and velocity fields that yield time histories of strain and kinetic energies that match the target systems. The proposed DDV method also serves as a procedure for restoring the eigenvalues and eigenvectors of a deficient dynamical system when known data is taken into consideration. Method is applied to smooth as well as non-smooth model problems and mathematical attributes of the formulation are investigated.

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Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THERMO-CHEMO-MECHANICAL MODEL AND VARIATIONAL MULTISCALE METHOD FOR MATERIAL AND GEOMETRIC EVOLUTION IN FRONTAL POLYMERIZATION

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ABSTRACT

This talk presents a new thermodynamically consistent model for thermo-chemo-mechanical processes in frontal polymerization. The model is comprised of nonlinear elastic solids undergoing large strains, and locally undergoing advancing reactive fronts as the material is extruded. The development of the formulation starts from balance equations for mass, momentum, and energy. The constitutive relations are derived to enforce non-negative entropy production to satisfy the second law of thermodynamics for the open system where mass is continuously added to the system. The model considers factors, namely, heat generation, heat transfer, and reaction kinetics that incorporate the rate at which the monomers are converted into polymers and the associated heat release. The material parameters evolve as a function of time to model chemical curing of the polymeric material. The coupled deformation due to thermal and chemical effects is carried out via a multiplicative split of the deformation gradient.

A stabilized finite element form that is derived based on the Variational Multiscale framework is presented, and the constitutive model is integrated in the VMS stabilized method. This leads to a fully coupled method for modeling and simulation of the thermo-chemical effects and localized curing at the propagating front. The VMS stabilized form helps circumvent the inf-sup condition commonly termed as the Babuska-Brezzi condition for mixed field problems, thereby allowing the use of arbitrary shape function for the displacement and temperature field. In addition, it also addresses the incompressibility constraint on the material that otherwise requires special stress projection methods or reduced integration techniques. A ghost mesh technique is proposed for extrusion printing of material, and a moving point is defined to represent the kinematics of the printing nozzle. At each step, integration points around the nozzle are activated and assigned the actual stiffness and density of the material to simulate extrusion of the material. The model and method are validated with experimental data, and some interesting test cases are presented.

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Deep and machine learning methodology in the context of application to computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREDICTION OF PRESSURE FIELD OF INCOMPRESSIBLE FLOW USNING CNN

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ABSTRACT

In the previous work, we proposed a prediction method of incompressible flow using ConvLSTM (Convolutional LSTM) based on pressure and velocity field of a couple of previous steps. To improve the proposed method, we have changed the procedure of the pressure prediction in which the pressure field of the current step and the velocity field of the next step (predicted by ConvLSTM as the same as the previous work) are given to CNN (Convolutional Neural Network), but not to ConvLSTM, as in Computational Fluid Dynamics (CFD), pressure field is solved by the Poisson equation which does not have a time derivative term. The results are compared with those obtained by the previous work.

Numerical modelling of composite materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ANALYSIS OF LAMINATED COMPOSITE AND SANDWICH PLATES SUBJECTED UNDER THERMO-MECHANICAL LOAD USING LEAST SQUARE FINITE ELEMENT MODEL

Christian Mathew[*1] and Yao Fu*[1]

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ABSTRACT

Combination of one or more Engineering materials on a macroscopic level produces composite. The composite materials have better engineering properties than parent materials individually. Laminated composites are widely used in many engineering industries such as aircraft and spacecraft, boat hulls, racing car bodies and storage tanks. This study presents the thermoelastic analysis of laminated composite plates subjected to sinusoidal thermal load (simultaneously loaded by mechanical and thermal loads) linearly varying across the thickness. Least square finite element solutions for thermal displacements and stresses are investigated by using a mathematical model, called a state-space model, that allows us to simultaneously solve for these quantities in the composite structure's domain and making sure that continuity conditions are satisfied at layer interfaces. We solve the governing equations that are derived from this model by using a numerical technique called the least-squares finite element method (LSFEM) which seeks to minimize the squares of the governing equations and the associated side condition residuals over the computational domain. Numerical results are presented to demonstrate the thermal response of the laminated composite plates using LSFEM and compared with three-dimensional elasticity solution available in the literature.

Industrial applications of IGA
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VANQUISHING MEMBRANE LOCKING IN QUADRATIC NURBS-BASED DISCRETIZATIONS OF NONLINEAR KIRCHHOFF-LOVE SHELLS: CAS ELEMENTS

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ABSTRACT

Continuous-assumed-strain (CAS) elements were recently proposed to remove membrane locking in quadratic NURBS-based discretizations of linear plane curved Kirchhoff rods [1] and linear Kirchhoff-Love shells [2] and shear and membrane locking in quadratic NURBS-based discretizations of linear plane curved Timoshenko rods [3]. In this work, we generalize CAS elements to remove membrane locking from quadratic NURBS-based discretizations of geometrically nonlinear Kirchhoff-Love shells. CAS elements are an assumed strain treatment. Leveraging the C1 continuity across element boundaries of the displacement vector given by quadratic NURBS, CAS elements bilinearly interpolate the covariant membrane strain coefficients at the knots resulting in assumed strains with C0 continuity across element boundaries. The benchmark problems show that CAS elements excise the spurious oscillations of membrane forces caused by membrane locking for an ample range of slenderness ratios. In addition to successfully vanquishing locking, CAS elements are a computationally efficient element type since no additional degrees of freedom are introduced, no additional systems of algebraic equations need to be solved, no matrix operations such as matrix multiplications and matrix inversions are needed, the nonzero pattern of the tangent matrix is maintained, and 2x2 Gauss-Legendre quadrature points suffice to integrate each element.

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Modeling mechanics of materials with voids
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING THE EFFECT OF BACKBONE INSTABILITIES AND GUEST OCCUPANCIES ON INTERFACIAL AND STRUCTURAL PROCESSES AND DYNAMICS OF SII GAS HYDRATE SYSTEMS USING MOLECULAR DYNAMICS

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ABSTRACT

Gas hydrates are inclusion compounds comprising a backbone of water molecules that enclose guest molecules in separate cages. Each volume of hydrate contains 160 volume equivalents of gas. Initially, large scale gas hydrate research was centered around the flow assurance problems they cause in the extraction and transportation of petroleum and its derivatives. Naturally occurring gas hydrates are also studied to satisfy global energy demand. Their potential use in the removal of carbon from the atmosphere, carbon capture and storage, and for energy exploitation makes gas hydrates a prime candidate for climate change mitigation research. At the atomic scale, these structures may be perfect crystals, but at the macroscale they will display imperfections. These can present themselves as missing water molecules in the hydrate backbone, and missing guest molecules in otherwise filled structures. Naturally, the properties of hydrates are centered around the formation and population of voids in the cage structure – the guest molecule's presence serves to stabilize the backbone and its absence may induce structural instabilities. This work uses molecular dynamics as implemented in the Large-scale Atomic/Molecular Massively Parallel Simulator to characterize the temperature and pressure effects on the interfacial tension, energy of interfaces, and growth rate of natural gas hydrates to overcome the complexity of experimentally understanding their performance in extreme environments and prove that theoretical modeling, prediction, and advanced characterization techniques can explain the structural and transport properties that govern hydrate in engineering applications. Additionally, this work will use the same techniques to study how behavior at the interface is affected by the presence of voids in the crystalline structure. It is essential to understand the underlying behavior of the hydrate cages to characterize the macroscale properties of real materials that are not perfectly filled crystals. Also, by studying the principal phases involved in hydrate formation, hydrate/water, hydrate/gas, and hydrate/ice, the work seeks to determine how the population of vacancies may be controlled by tuning surface behavior during the melting and formation processes. Preliminary results confirm the presence of a novel pre-melting layer at the interface between structures that shows strong atomic alignment behaviors. Detailed dipole analysis shows that some tuning may be performed with external forces to change the transport properties through this layer. Combined with changes in temperature and pressure, voids in the background structure may be avoided or preferred, while achieving control of the cage populations.

Advanced model order reduction techniques for computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PARTICLE-BASED REDUCED ORDER MODELING OF LAGRANGIAN FREE SURFACE FLOW USING DEEP LEARNING

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ABSTRACT

Reduced order modelling (ROM) is a method to solve time evolution int a low-dimensional space and is widely used for control and optimization problems, since it can predict physical fields quickly. Deep learning models have been used to emulate the ROM. One of recent models allows order reduction while maintaining spatial continuity of the physical field, allowing it to handle large datasets such as meshes and point clouds [1]. This function allows it to be applied to problems involving Lagrangian particle tracking, particularly in scenarios such as free surface flows, which pose difficulties for conventional ROM. Deep learning-based ROM can be divided into the learning phase, where order reduction and reconstruction is learnt, and the prediction phase, where time evolution is performed on the low-dimensional space. In the prediction phase, time variables are evolved in time on a coded low-dimensional space using either prediction by a learning machine or iterative optimization with the governing equations as residuals. The latter is preferable to avoid the black-boxing of deep learning, but for problems where particles move in a Lagrangian description, the computational cost of the derivatives is high and iterative optimization with the governing equations as residuals is difficult. Then, the objective of this study is enhancing computational performance of deep learning-based ROM for free surface flow. To approach this problem, it is proposed to decode all physical values simultaneously and optimizing time-varying variables in low-dimensional space based on a comparison of explicitly calculated and decoded velocities. By encoding all physical quantities simultaneously, time evolution based on one physical quantity can also be used to time evolve other physical fields. Also, time evolution based on residual computed by explicitly calculated and decoded velocities eliminates the need to calculate residuals based on the governing equations every step in an iterative calculation. These methods were validated on a dataset of the water drop problem created by the SPH method. As a result, it is confirmed that the proposed decoding method can reduce order and reconstructed original physical field well and proposed optimization method can reduce computational const than the model proposed in previous studies.

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Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN ADAPTIVE SPACETIME WAVELET METHOD FOR PREDICTIVE COMPUTATIONAL SCIENCE WITH MULTIPLE SPATIAL AND TEMPORAL SCALES

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ABSTRACT

Modern computational science and engineering applications are inherently multiphysics and multiscale. Therefore, novel algorithms are required to solve nonlinear Partial Differential Equations (PDEs) with features evolving over a wide range of spatial and temporal scales. In this work, we propose a wavelet-based method that is ideally suited for problems developing localized structures, which might occur intermittently anywhere in the computational domain or change their location and scales in space and time. Wavelets have generated tremendous interest in both theoretical and applied areas as they allow for efficient multiscale decomposition and large data compression. In our work, we develop the Multiresolution Wavelet Toolkit (MRWT), which requires far fewer unknowns than other algorithms when applied to problems with a great range of spatial and temporal scales. In addition, the computational grid can be refined locally, and our a priori error estimates safeguard the accuracy of the numerical solution.

MRWT has been implemented as a hybrid parallel framework using a modern programming paradigm to execute in a hybrid CPU/GPU environment. Consequently, MRWT provides high-fidelity simulations with significant data compression. We explain how this technique uses differentiable wavelet basis functions and second-generation wavelets to solve nonlinear PDEs on finite domains. Moreover, we provide a priori error estimates for the wavelet representation of fields, their derivatives, and the nonlinear terms in PDEs. Additionally, MRWT utilizes a predictor-corrector procedure within the time advancement loop to dynamically adapt the computational grid, retaining the prescribed accuracy of the solutions of the PDEs as they evolve. First, we employ an embedded Runge-Kutta (RK) integration scheme to control the temporal accuracy as the solution of the PDE advances. Second, we will also present a novel spacetime method and solve the full spacetime problem using adaptive wavelets. Our preliminary spacetime results on dense grids show promise for the development of sparse spacetime wavelet schemes.

We show rigorous verification of the MRWT algorithm for both time marching (RK integration) and spacetime problems, demonstrating mathematical correctness and physics simulation capabilities. Furthermore, we show that we achieve spatial convergence at a rate that agrees with a priori estimates. Whereas traditional numerical techniques require a sequence of solutions on multiple grids (i.e., solution verification), our adaptive wavelet method provides self-verification from a single simulation. Finally, we apply MRWT to problems with shocks in gases using compressible Navier-Stokes equations and to high-strain rate damage nucleation and propagation in nonlinear solids using Eulerian-Lagrangian dynamic damage modeling.

Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFECT OF THE INELASTIC SELF-HEATING ON THERMO-MECHANICALLY COUPLED TWO-SCALE BEHAVIORS

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ABSTRACT

Thermo-mechanically coupled behaviors of polymer composites are challenging phenomena that are difficult to measure experimentally but critical issues in their design and manufacturing[1]. The viscous property in their matrix materials not only causes their temperature-dependent mechanical behavior but also generates the heat source by the inelastic energy dissipation. Such an inelastic self-heat acts as an instantaneous heat source, so that the unsteady thermo-mechanically coupled behavior emerges in their microstructure, which may be impossible to analyze overall responses experimentally. The conventional computational homogenization methods for thermo-mechanically coupled problems[2] are also not applicable to this problem because the unsteadiness disappears in an infinitely small unit-cell. For this reason, few researchers have comprehensively studied the effect of inelastic self-heating on the two-scale thermo-mechanically coupled behaviors in dissipative composites.

We formulate a thermo-mechanically coupled two-scale boundary value problem for dissipative composites and establish a method of two-scale analysis to capture the transient thermo-mechanically coupled behaviors caused by the inelastic self-heating. Under the assumption of a real-size unit-cell[3], the approximative two-scale decomposition and the suitable linearization for a coupled rate potential stored of dissipative composites yield governing equations that characterize the mutual relationship between mechanical equilibrium and unsteady heat conduction in both scales. We show that the periodic boundary condition for the microscopic temperature is only available to simulate transient two-scale behaviors, which is consistent with the results of single-scale analysis. The effect of inelastic self-heating on the transient two-scale behaviors is comprehensively studied through several numerical examples for plastic and viscoplastic composites.

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Fluid-structure interaction in interface and moving boundary problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT OF A MESH-CONSTRAINED DISCRETE POINT METHOD FOR MOVING BOUNDARY FLOW PROBLEMS

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ABSTRACT

A particle-based method is a practical tool for simulating particle-laden flows. In recent years, novel types of methods have been proposed that guarantee convergence accuracy based on applying a moving least-squares (MLS) approximation (e.g., [1]). One of the disadvantages of the Lagrangian-type formulation is to encounter a sparse or dense arrangement of the particles even though an incompressible flow field is solved. Regarding this, an arbitrary Lagrangian-Eulerian (ALE) formulation has been implemented (e.g., [2]). However, since the particles at moving boundaries are tracked in a full Lagrangian manner, some problems have still remained for high computational efficiency and difficulty in parallel computations, which are attributed to the nonuniform distribution of particles and the update of their local arrangement over time. To tackle these problems, we have developed a novel particle-based (or meshless) method, termed mesh-constrained discrete point (MCD) method [3], in stationary boundary problems. A spatial discretization of the MCD method relies on the generalized finite difference method, a meshless method using the MLS approximation; however, the arrangement of particles (or discrete points (DPs)) is specialized, where their positions are constrained by background meshes to obtain a closely uniform distribution for the DPs even though an arbitrary boundary interface is immersed in an analysis domain. This achieves a reasonable approximation for spatial derivatives with compact stencils without encountering any ill-posed condition and would also lead to high computational efficiency. In this study, we develop the MCD method for coupled problems between an incompressible fluid and rigid bodies, where the ALE formulation is applied. To ensure the mesh constraint of each DP in moving boundary problems, the position of DPs is not only rearranged but also reassigned the role of being on the boundary or not. The developed method shows reasonable results in numerical experiments for both enforced displacement problems and fluid-solid interaction problems.

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Computational methods in environmental fluid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GAS-LIQUID-SOLID THREE-PHASE FLOW ANALYSIS WITH MULTIPLE OBJECTS USING FINITE ELEMENT METHOD

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ABSTRACT

Numerical method of multi-phase-field model three-phase analysis in gas, liquid and solid using tetrahedron (unstructured grid) is investigated. The Multi-Phase-Field model employs the Cahn-Hilliard equation [1] with multiple objects. In this study, we propose a mixed finite element method with MINI element considering implicit method in time direction and stabilization in space direction [2]. In this paper, the Cahn-Hilliard equation with multiple objects is used as a gas-liquid solid by the multi-phase-field three-phase model, and the fall computation of the structure is performed as a computational example to show the effectiveness of the proposed method.

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Recent advances in meshfree and particle methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PARTICLE SUSPENSION FLOW MODELING IN MOVING PARTICLE HYDRODYNAMICS

Kyuya Matsumoto[12], Shu Hiramoto[2], Masahiro Kondo[1], Tomohiro Sawada[1], Junichi Matsumoto[1], Kazuya Shibata[2] and Hideaki Nakajima[1]*

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ABSTRACT

In this study, we present a novel modeling of particle suspension flow in the moving particle hydrodynamics (MPH) [1, 2]. Suspension flow and particle transport are important in the tape casting process used in the manufacture of ceramic capacitors, piezoelectric devices, and solid all solid-state batteries. Particle methods have advantages over mesh methods (e.g. finite volume methods) in dealing with the fluid-solid interface in suspension flows. For example, particle methods do not require a mesh and do not require complex processing due to the mesh. In this study, we present a new modeling of suspension flow using the MPH. Each solid particle in a suspension flow is represented by a group of extremely viscous fluid particles. Compared to the existing methods based on the explicit incompressible SPH, such as the method of Bian et al. [3], the proposed method has the advantage of being able to compute highly viscous fluids without being limited by the diffusion number and to compute the motion of solid particles in the fluid in a unified fluid calculation. This is due to the fact that MPH implicitly updates velocities and preserves linear and angular momentums. The presented method can simulate not only Newtonian fluids but also Hershel-Bulkley fluids.

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PSE (Problem Solving Environment)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT OF A REMOTE LEARNING SUPPORT FRAMEWORK UTILIZING VIDEO ANALYSIS AI

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ABSTRACT

In recent years, various ICT education environments have undergone significant development, with the widespread adoption of video systems bringing about transformative changes in education. Enhancing the learning environment to effectively support distance education has become increasingly crucial.
In this study, we present the development of a comprehensive framework comprising a server system implemented within a web-based operating environment and a content creation support system. The system integrates multimedia content delivery functionality through a combination of a Web server and a game engine. Acting as a portal for lecture content, a reverse proxy is deployed, and Python Flask is utilized for user management to delegate functionality. The use of a template engine for delivering lecture content is aimed at achieving a streamlined and lightweight design, ensuring rapid response times. Moreover, the system captures close-up images of students through a webcam connected to the client, enabling various functionalities, including emotion analysis, skeletal estimation, and recording vital data such as heart rate measurements derived from detected facial images. This feature facilitates the analysis of user emotions. The developed system successfully establishes a platform that supports remote lecture delivery. Future efforts will focus on utilizing the framework for both remote and in-person classes. Recognizing the large file sizes of multimedia content, the system is designed for operation on Wi-Fi/5G, with the assumption of a LAN environment. Additionally, by monitoring participants through the implemented emotion analysis feature, we aim to contribute to the creation of more engaging and enriching educational content.

Computational methods in environmental fluid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TWO-DIMENSIONAL RIVERBED VARIATION ANALYSIS USING DISCONTINUOUS GALERKIN METHOD WITH SEDIMENT TRANSPORT EQUATION

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ABSTRACT

In recent year, global warming has caused river inundation and storm surge on a global scale. Numerical simulation of damage prediction is strongly demanded for planning mitigation or prevention from these natural disasters. Shallow water equations (SWEs) can decrease numerical simulation cost keeping with its accuracy, and simulation tools based on the SWEs are widely used for these natural disaster simulations. In shallow water flow analysis, stabilized finite element methods that introduce upstreaming, such as the SUPG (Streamline upwind/Petrov-Galerkin) method, have been widely used due to numerical instabilities caused by the fact that the SWEs are hyperbolic partial differential equation [1].
On the other hand, a discontinuous Galerkin (DG) method [2] is effective and promising tool for the hyperbolic equations with discontinuities. The DG method has been applied and shown to be effective in the shallow water flow analysis recently [3]. However, there are few precedents for such analysis using the DG method, although riverbed variation analysis that considers sediment erosion and deposition in the river channel is necessary to accurately predict damage such as river flooding.
In this study, the DG method is applied to riverbed variation simulations, in which the governing equation are coupling of the SWEs and equilibrium sediment transport equation. Then, we confirmed the validity of the proposed method has been verified with numerical analysis such as erodible dam-break flow and sandbar migration simulation.

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Recent advances in meshfree and particle methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A COMPARATIVE STUDY OF CONVENTIONAL AND ADVANCED PARTICLE METHODS ON RESULTANT ACCURACY AND COMPUTATIONAL COST

Takuya Matsunaga[*1] and Hiroshi Okuda*[1]

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ABSTRACT

Particle methods have received a great deal of attention in various scientific and engineering fields because of their remarkable capabilities in simulating complicated fluid flow problems such as free-surface flows with splash generation. The smoothed particle hydrodynamics (SPH) method and moving particle semi-implicit (MPS) method are the two most widespread particle methods with which a considerable number of studies have been conducted for over a decade. However, these traditional particle methods employ inconsistent discretization schemes, and ensuring the reliability of numerical results has been a major problem.

With this background, enhancing the accuracy of particle methods has been one of the main topics of active research. One of the most notable developments in this context is the least squares moving particle semi-implicit (LSMPS) method (Tamai and Koshizuka, Comput. Part. Mech., vol. 1, pp. 277–305, 2014). The LSMPS method is characterized by its highly accurate spatial discretization scheme. In a recent study, the authors have improved the numerical stability of the LSMPS method by incorporating several numerical techniques and proposed the stabilized LSMPS method (Matsunaga and Koshizuka, Comput. Methods Appl. Mech. Eng., vol. 389, p. 114416, 2022). The stabilized LSMPS method can be applied to complex free-surface flow problems in the same way as the conventional SPH and MPS methods.

In this presentation, several specific applications of the stabilized LSMPS method are presented in comparison with the conventional MPS method, demonstrating its effectiveness for highly accurate numerical simulations and providing insight into the feasibility of practical applications. More specifically, we show that significant differences are observed between the results of the two methods, particularly in problems where negative pressure plays an important role in fluid motion. Furthermore, we show that the method is highly effective also for the analysis of highly viscous fluids and surface tension flows. In addition, we compare the computation time to provide quantitative information on how much the computational cost increases when the conventional method is replaced by the stabilized LSMPS method.

Modeling, optimization and computational analysis of metamaterials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NON-HERMITIAN DEGENERACY IN TWO-DIMENSIONAL OPEN ELASTIC SYSTEMS WITH HIGHER-ORDER EXCEPTIONAL POINTS

Kei Matsushima[*1] and Takayuki Yamada*[1]

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ABSTRACT

In this talk, we present a numerical model of two-dimensional solid structures with cylindrical symmetry and demonstrate the existence of higher-order exceptional points in the elastic system. Elastic waves propagating in the system are subject to radiation loss, resulting in their associated eigenvalues becoming complex-valued. By tuning certain system parameters, we numerically demonstrate the simultaneous coalescence of complex eigenvalues and their corresponding eigenmodes. Our numerical experiments suggest that this non-Hermitian degeneracy stems from (higher-order) exceptional points in the parameter space. We expect that this discovery opens the possibility for a novel technique in mechanical sensing.

HIGH-FIDELITY SIMULATIONS OF LOWFREQUENCY SOUND IN REAL 3D APPLICATIONS

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ABSTRACT

We have developed a high-fidelity numerical model to accurately simulate sound propagation in a realistic, stratified and windy 3D atmosphere over irregular terrain. In particular we are interested in low frequency sound propagation from large windfarms. The numerical simulations are validated against accurate measurements of sound pressure levels (SPL) all the way down to 1 Hz. Comparisons is done also against the most commonly used community sound propagation models in Sweden such as NORD2000. A previous study showed that some of the most commonly used methods for environmental noise [1] failed completely to predict the correct SPL in irregular terrains. The reason for this is related to the fact that they do not take the underlying physics into consideration and instead involve ad. hoc. tuning of non-physical parameters.

Outdoor sound propagation is highly affected by ground effects, refraction and damping in the atmosphere, topography, the sound power levels and relative positions of the sound sources [2]. To accurately simulate outdoor sound propagation requires a careful consideration of the underlying physics and good knowledge of the uncertainties in model data. Obtaining a stable and accurate solution of the 3D high-fidelity sound propagation model, in this case the acoustic wave equation, is a nontrivial task.

The huge computational 3D domain, and the need to accurately resolve low-frequency waves require the use of high-order accurate numerical methods, having minimal dispersion (and dissipation) errors. A robust and well-proven high-order finite difference methodology, for well-posed initial boundary value problems is to combine summation-by-parts (SBP) operators [3] and the simultaneous approximation term (SAT) method to impose boundary conditions (BC). This is the methodology adopted in the present study. In an effort to significantly reduce computational times the numerical SBP-SAT method is implemented on GPUs, resulting in relatively short simulation times, despite large degrees of freedom.

Uncertainties in (atmospheric, terrain and source characteristic) data is analyzed using uncertainty quantifications, which allow for reliable error bounds on the prognosis of SPL in the far field.

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SciML in the real world
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-ASSIMILATION FOR NUMERICAL WEATHER PREDICTION WITH SCIENTIFIC MACHINE LEARNING

Matthew Poska[1], Alexander Wikner[2], Rao Kotamarthi[3], Troy Arcomano[3] and Romit Maulik[*1]*

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ABSTRACT

Data assimilation (DA) in geophysical sciences remains the cornerstone of robust forecasts from numerical models. Indeed, DA plays a crucial role in the quality of numerical weather prediction and is a crucial building block that has allowed dramatic improvements in weather forecasting over the past few decades. DA is commonly framed in a variational setting, where one solves an optimization problem within a Bayesian formulation using raw model forecasts as a prior and sparse experimental observations in a likelihood. In traditional DA, the forward model is numerically and computationally expensive. Here we replace the forward model with a differentiable surrogate model. Consequently, gradients of our DA objective function with respect to the decision variables are obtained rapidly via automatic differentiation. We use our proposed method for assimilating radiosonde observations for improved numerical weather prediction using a vision transformer surrogate. Our results indicate that emulator-assisted DA is faster than traditional equation-based DA forecasts by 4 orders of magnitude, allowing computations to be performed on a workstation rather than a dedicated high-performance computer.

Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VALIDATION OF DISPLACEMENT DAMAGE MODELS

Kathryn Maupin[*1], Jaideep Ray[1], Larry Musson[1] and Suzey Gao[1]*

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ABSTRACT

As the third pillar of science, computational simulation has allowed scientists to explore, observe, and test physical regimes previously thought to be unattainable. High-fidelity models are derived from physical principles and calibrated to experimental data. However, missing or unknown physics and measurement, experimental, and numerical errors give rise to uncertainties in the model form and parameter values in even the most trustworthy models. Thus, rigorous calibration and validation of a computational model is paramount to its effective us as a predictive tool. The popularity of the Bayesian paradigm stems from its natural integration of measurement and model uncertainties. A systematic approach to model validation, as originally outlined by Oden, et al in [1-2], progressing from parameter and quantity of interest identification to sensitivity analysis, calibration, and validation, is applied to a drift-diffusion simulation code called Charon. Charon allows the computational qualification of semiconductor devices subjected to displacement damage. This work is dedicated to Dr. J. Tinsley Oden.

*Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration
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BAYESIAN OPTIMAL DESIGN OF PULSED POWER EXPERIMENTS

Kathryn Maupin[*1] and Chris Jennings*[1]

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ABSTRACT

Traditionally, there are two pillars of science: theory and experimentation. These two inform one another and lead scientists to make educated guesses and decisions toward advancing science. More recently, the driving force behind scientific advancement has not just focused on how much information can be learned, but how quickly. Additionally, experimental data can be costly and difficult to obtain. With these motivations in mind, the field of experimental design aims to maximize the information gained from as few experimental data points as possible. Computation has emerged as a third pillar of science to complement the traditional two and has been used to facilitate optimal experimental design. However, missing or unknown physics as well as measurement, experimental, and numerical errors give rise to uncertainties in model output in even the most trustworthy models. These uncertainties are effectively acknowledged and incorporated during a Bayesian analysis. However, in many practical applications, high-fidelity physics-based codes are intensive, making them infeasible to use directly in design and optimization studies. To preserve confidence and capture uncertainties in these studies, it is imperative that surrogate or reduced order models accurately capture available data.

Sandia's Z machine is the world's most powerful and efficient laboratory radiation source. Z experiments often exhibit large current losses, so a principal uncertainty is how effectively current can be delivered. Power flow simulations are very intensive, making them infeasible to use in critical design and optimization studies. Generator and target design necessarily rely on highly-reduced circuit models with simplified current loss terms informed by Z experiments. However, incomplete experimental time histories and rigorous calibration and validation of surrogate models limit accurate constraints and introduce uncertainties into the characterization of loss processes. Developing a consistent picture of how losses develop and evolve would improve understanding of present-day experiments and better constrain circuit model representations, providing a basis for quantifying uncertainties in circuit models applied to Z and improve confidence in predictions of target performance. This presentation details the implementation of a Bayesian optimization study to maximize the information gained from Z experimental data and design.

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Modeling and simulation of advanced manufacturing processes for metals
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DISTORTION MODELING OF PM HIP PARTS PRODUCED WITH AM HIP CAPSULES

Jason Mayeur[*1], Soumya Nag[1], Fred List[1] and Peeyush Nandwana[1]*

[1]Oak Ridge National Laboratory

ABSTRACT

Fabricating components via PM HIP is a well-established process capable of producing high quality near net shaped parts with excellent material properties. The process has been widely adopted by the offshore oil and gas industry and is increasingly being explored as an alternative process to make large parts for other energy sectors (e.g., nuclear, hydroelectric) to alleviate supply chain issues associated with large scale castings and forgings. The primary bottleneck of producing parts through the PM HIP route is the design and fabrication of the HIP capsule. HIP capsules are currently fabricated by hand through working and welding of sheet metal to produce the required capsule geometry, which can be a tedious process for complex geometries. To this end, there is interest in exploring the feasibility of fabricating HIP capsules via additive and/or hybrid manufacturing processes, which can drastically reduce capsule fabrication time. It is well known that the mechanical properties of AM materials may differ substantially from their wrought counterparts due to microstructural differences. Therefore, AM HIP capsules may present some challenges during the capsule design process related to mechanical property variations and/or anisotropy. In this study, we compare and assess the consolidation behavior of a PM HIP component using both conventional and AM HIP capsules and use a finite element model to understand the differences in consolidation behavior between the two cases.

Fracture, damage and failure mechanics of cementitious materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADVANCED NUMERICAL MODELING OF CONCRETE IN MESO-SCALE

Gianluca Mazzucco[*1], Beaudin Beaudin[1], Beatrice Pomaro[1], Jiangkun Zhang[1], Valentina Salomoni[1] and Carmelo Majorana[1]*

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ABSTRACT

Numerical modeling of concrete poses distinctive challenges owing to its nonlinear behavior, encompassing both hardening and softening characteristics. Undertaking long-term investigations further complicates matters, necessitating the precise representation of damage, creep, and fatigue [1]. This complexity adds layers to the already intricate processes of material characterization and modeling. Concrete is widely employed in diverse engineering applications, frequently entailing intricate multi-physics phenomena. These applications demand sophisticated numerical tools to ensure reliable predictions of associated state variables.
This study introduces a numerical approach focused on modeling cementitious materials at the constituent level. Specific constitutive laws are employed for the cement paste and aggregates, while the Interfacial Transition Zone (ITZ) is delineated using a cohesive algorithm [2]. The creation of realistic solid concrete models at the mesoscale is addressed through the utilization of advanced random distribution techniques and Computed Tomography.

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Fluid dynamics and SciML: Navigating challenges and seizing opportunities
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

REALIZABILITY-INFORMED LEARNING OF DATA-DRIVEN TURBULENCE MODELS

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ABSTRACT

Traditional turbulence closure models for Reynolds-Averaged Navier-Stokes (RANS) simulations rely on a mixture of physics-based intuition and heuristics. Recently, the application of machine learning towards replacing components of a closure model, or replacing the closure model entirely have attracted significant interest. Data-driven techniques offer a promising alternative to traditional closure modelling, since they offer the ability to leverage data from high fidelity numerical simulations to increase the accuracy of turbulence models for RANS. RANS remains an important and widely used technique for industrial users. Perhaps the most important issue for data-driven closure modelling is the issue of generalizability. Traditional physics-based closure models can generalize to a variety of flows. However, modern data-driven RANS closure models do not generalize well. In other words, though data-driven methods improve the accuracy of RANS simulation on similar flows to the training dataset, they do not make reliable predictions on flows that are significantly different than the training dataset.

The objective of the present study is to propose and demonstrate multiple techniques to increase the generalizability of data-driven closure models. A key issue among all modern data-driven RANS closure models is that they do not guarantee a realizable anisotropy tensor. Physical realizability is a constraint on the anisotropy tensor which arises from requiring the symmetric Reynolds stress tensor to be positive semi-definite. Since the training procedure for most data-driven closure models usually involves a simple mean squared error (MSE) or mean absolute error (MAE) loss function, the models often make unrealizable predictions. The most common technique to address this issue is to post-process the predictions using ad-hoc methods.

We propose the inclusion of a term in the loss function which penalizes unrealizable predictions at training time, thereby embedding additional physics-based information into the model. Along the lines of physics-informed machine learning, we term this technique realizability-informed learning. In the work to be presented at WCCM 2024, we will demonstrate that this penalty term reduces prediction error on new test cases, thereby demonstrating that realizability-informed learning enables data-driven closure models to generalize better. We will also demonstrate that a model trained using realizability-informed learning makes more realizable predictions that a model trained using a purely error-based loss function. In doing so, we aim to simultaneously address two key issues for data-driven closure models: making more realizable predictions, and improving the generalization of the model outside of the training dataset.

Constitutive modeling of complex materials with machine learning and artificial intelligence
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SPARSE REGRESSION, LP-REGULARIZATION, AND AUTOMATED MODEL DISCOVERY

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ABSTRACT

Sparse regression and model discovery are essential to gain physical insight from large amounts of data. These techniques allow us to discover interpretable and predictive models that provide simple relationships among scientific variables. While the statistical tools for model discovery are well understood in linear regression, their extension to nonlinear regression is often domain-dependent and can be computationally challenging. Here we integrate physical constraints and regularization to extract interpretable strain energy functions from mechanical testing data [1]. In particular, we used constitutive artificial neural networks to ensure that we discover models that satisfy known material symmetries and thermodynamic laws, and we used Lp regularization to reduce the number of parameters in the model [2]. We trained our networks on both synthetic and experimental data and observed the following trends: L2 ridge regularization fails to increase sparsity; L1 lasso regularization improves sparsity but introduces significant bias in the resulting parameters that hinders accuracy; L0.5 and L0 regularization allow us to fine-tune the trade off between interpretability and accuracy, but can be challenging to implement as the model complexity increases. With these insights, we demonstrated that constitutive neural networks can discover highly accurate parsimonious models with a few nonzero parameters. Our ability to discover interpretable constitutive models from data has the potential to provide physical and physiological insight into the mechanical properties of living systems. These insights can enable better understanding of disease progression, and can also allow for the development of better biomaterials. We expect that our results will generalize to other model discovery techniques, and to other fields including biology, chemistry, and medicine.

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Towards predictive digital twins: Innovative algorithms for physics-, data-assisted and hybrid modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BAYESIAN LEARNING OF REDUCED-ORDER OPERATORS WITH GAUSSIAN PROCESSES

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ABSTRACT

This work presents a data-driven method for learning reduced-order models whose predictions are endowed with uncertainty estimates. The operator inference approach to model reduction poses the problem of learning reduced-order model operators as a regression of state space data and corresponding time derivatives. When time derivative data are not natively available, as is often the case in applications, they must be estimated from the state data with, e.g., finite difference approximations. The accuracy of the estimation greatly affects the quality of the learned reduced-order model, hence learning accurate reduced-order models in this manner is challenging when available state data are sparse or noisy. Our approach incorporates Gaussian process surrogate modeling into the operator inference framework to (1) probabilistically describe uncertainties in the state data and (2) procure analytical time derivative estimates with uncertainty. The formulation leads to a generalized least-squares regression and, ultimately, reduced-order operators that are themselves defined probabilistically. The resulting model propagates uncertainties from the observed state data to reduced-order predictions.

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New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SHAPE AND TOPOLOGY OPTIMIZATION OF COMPOSITE COMPLIANT MECHANISMS ACTIVATED BY PIEZOCERAMICS

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ABSTRACT

This work aims to develop a formulation based on topology optimization technique for designing compliant mechanisms activated by piezoceramics. The novelty of the work is that not only the passive mechanism body, but the piezoelectric material shape is synthesized as well. Therefore, the actuator shape is studied together with the complaint mechanism. Another novelty of the work is that the passive material is made of composite material, having different mechanical behavior depending on the reinforcement orientation. The importance of designing such mechanisms is that piezoelectric actuators can be used in various applications, including embedded electronics and medical equipment, both requiring applications at micro and nanoscales. At these scales, compliant mechanisms have a clear advantage over other devices since they are built from one material layer, therefore are free of hinges and joints, minimizing the appearance of backlash and clearance when several cycles of application are required. The proposed formulation considers the active and passive material of the mechanism materials set in the topology optimization problem. The goal is to design mechanisms with a more efficient displacement transfer from the input to the output ports. The domain is discretized using the finite element method assisted by the implementation of Python libraries through FEniCS (Finite Element Computational Software) project and the derivatives are computed numerically using dolphin adjoint packages. Material interpolation scheme for the topology optimization problem is applied by means of the PEMAP (PiezoElectric Material with Penalization) method [1] that is a variant of the so-called SIMP (Solid Isotropic Material with Penalization) with the advent of extra terms that consider the piezoelectric effect in the active material phase. The optimization problem to be solved in this work is a multi-objective problem of minimizing mean compliance and maximizing mean transduction. The mathematical solver implemented is the so-called MMA (Method of Moving Asymptotes). Results show that the methodology applied works successfully for the examples with different polarization profiles.

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Data-driven modeling and design of materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

UNVEILING AMORPHOUS MICROSTRUCTURAL FEATURES: A MANIFOLD LEARNING APPROACH USING DIFFUSION MAPS

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ABSTRACT

Amorphous solid failure originates from local plastic rearrangements in the atomic configurations of the material during shear-induced deformation. By assessing the incremental stress needed to cause a local rearrangement, the Local Yield Stress (LYS) approach was recently developed to probe local regions and quantify their susceptibilities to plasticity. Despite its promising potential to deepen our insights into plastic deformation in amorphous solids, the method's computational demands limit its feasibility for predictive modeling. We propose a manifold learning-based framework to extract microstructural descriptors from atomistic configurations. More specifically, we deploy Diffusion Maps (DMaps, a nonlinear manifold learning technique) to systematically extract low-dimensional structural features from high-dimensional atomic configuration data. We then aim to relate this structure to material performance assessed by the LYS approach. In this manifold learning method, each data point corresponds to a geometric neighborhood of atoms, and thus a meaningful similarity measure between configurations must capture the “distance” between two neighborhoods. We utilize the newly developed Gaussian Integral Inner Product (GIIP) to measure this similarity, addressing important issues such as noise sensitivity, continuity, smoothness, permutation, and rotational invariance, making it robust for measuring similarity in randomly distributed atomic structures. We apply this method to a two-dimensional binary glass-forming system to characterize the local structure in the material, linking the diffusion coordinates from a neighborhood to well-known structural descriptors and new localized material performance measures. For example, we predict Conventional bond orientational order ($\Psi 5$, $\Psi 6$) and Generalized bond orientational order(Θ) with Gaussian Process Regression, showcasing the method's effectiveness in revealing the underlying structure. These relations have the potential to enhance our understanding of the complex interplay between microstructure and mechanical behavior in amorphous materials.

Mesh-free particle methods for multi-physics problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MACHINE-LEARNING-ENABLED SOLID BOUNDARY CONDITIONS IN MESH-FREE PARTICLE METHODS

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ABSTRACT

Meshfree particle methods such as Smoothed Particles Hydrodynamics (SPH) and Moving Particles Semi-Implicit (MPS) have become more popular in the simulation of flows with large interfacial deformations and fragmentations. These techniques use a kernel smoothing process to discretize the governing equations over the physical domain, represented by a set of free-to-move computational nodes called particles (Jandaghian, Krimi et al. 2021). Solid boundary conditions pose a challenge in these methods, primarily due to the near-boundary kernel incompleteness, which can negatively affect conservation properties. Various techniques are used to address solid boundaries in particle methods, including ghost (virtual) particles, mirror particles, boundary force, and polygon boundary conditions (Herman Musumari Siaben, Rubens Augusto Amaro Junior et al. 2023). While some of these methods have proven effective, their implementation presents challenges and is often computationally expensive, particularly when dealing with large-scale and complex geometries. This study introduces a novel machine learning (ML) technique for the implementation of solid boundaries in particle methods. Two distinct approaches are explored. The first approach develops a neural network (NN) to establish a relationship between geometric characteristics and boundary contributions within each MPS/SPH approximation operator. These include interpolation, gradient, divergence, and laplacian operators. In the second approach, a NN is designed to correlate geometric features with the total boundary contribution, specifically in SPH/MPS approximations of mass and momentum conservation in the Navier-Stokes equation. The ghost particle approach is used to generate a comprehensive training dataset of boundary contributions for various geometrical features. The trained models are subsequently tested in flow simulations involving diverse geometries. The results demonstrate the effectiveness of the developed approaches, with a significant computational cost reduction compared to the conventional ghost particle method.

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Computational mechanobiology of musculoskeletal tissues
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RANDOM WALK AND CONTINUUM MODELS FOR THE PROPAGATION OF BONE ADAPTATION SIGNALS THROUGH THE OSTEOCYTE NETWORK

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ABSTRACT

The adaptation of bone tissue to mechanical loads and the repair of bone micro-damage rely on the propagation of signaling molecules through the osteocyte network embedded in bone tissue. Osteocytes form a dense cellular network in bone able to sense mechanical deformation of bone tissue [1,2]. They regulate bone adaptation and regeneration by emitting biochemical signals that propagate through the network to the bone surface where they induce bone resorption and bone formation. How these biochemical signals propagate in bone is influenced not only by network topology but also by the spatial arrangement of osteocytes within bone tissue. Understanding the collective reaction-diffusion properties of these signals is important to evaluate when and where bone formation and bone resorption are initiated.

In this study, we explore stochastic and deterministic random walk models of signaling molecules propagating and reacting within osteocyte networks with various spatial arrangements of osteocytes and various osteocyte connectivities. By taking a continuum limit of the random walk models, we derive inhomogeneous reaction–diffusion–advection equations, where diffusivity and advective velocity depend on the local osteocyte density and connectivity within the network. Our findings reveal that heterogeneous osteocyte distributions induce large spatial variations in signaling molecule concentrations and influence their collective transport properties. Furthermore, we observe that noise within the stochastic random walk model is directly influenced by osteocyte density. We explore signal-to-noise ratios for different damage detection scenarios and demonstrate that the location of perturbations to the osteocyte network, representing micro-damage, can be detected by signals received at the network boundaries [3]. Finally, we apply this model of signal propagation to formulate a model of dynamic bone tissue with an evolving embedded osteocyte network, in which bone formation and bone resorption are controlled by osteocyte-generated biochemical signals received at the bone surface.

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Emerging topology and shape optimization techniques in computational design of materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DESIGN OF A SOFT PNEUMATIC ACTUATOR USING TOPOLOGY OPTIMIZATION AND POROHYPERELASTICITY

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ABSTRACT

This work presents a novel nonlinear topology optimization formulation as a tool for the computational design of pneumatically triggered soft actuators. Soft robotic actuators, typically made of elastomers, undergo very large deformations which can be simulated by the theory of hyperelasticity. Pneumatic actuators produce the desired output motion by pressurizing certain cavities in the structure, thereby loading the surrounding elastomer solid. In a computational setting, this pressurization can be modelled by the Darcy flow equations, with high permeability in cavities and low permeability in solid regions. Hence, a model is necessary that includes both Darcy flow and hyperelasticity in the entire design domain, with stiffness and permeability coefficients that depend locally on the design variable. In the present work, the two-field porohyperelasticity theory by Simon et al. (1996) is adopted, where displacement and pressure fields are both used as primary variables. Porohyperelasticity extends the validity of the Darcy flow and elastic deformation equations to configurations that exhibit very large deformation. This is a major improvement compared to the linear poroelasticity topology optimization formulation previously introduced by Kumar et al. (2021). We combined the permeability interpolation and drain term proposed by Kumar et al. (2021) with the porohyperelasticity formulation by Simon et al. (1996), and the nonlinear topology optimization framework with void regularization by Bluhm et al. (2023), in order to create an efficient, accurate, and generic computational framework for soft pneumatic actuators. The proposed formulation has been used to maximize the bending response of a 3D tube segment under certain external resistance, obtaining optimized designs which can serve as building blocks for constructing, e.g., gripper fingers and dexterous endoscopy tubes. The obtained 3D designs, although topologically similar to classical human-engineered solutions, achieve better controllability through their higher geometric complexity.

Keywords: Pneumatic soft robotics, nonlinear topology optimization, porohyperelasticity

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Imaging-based methods in computational medicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CHARACTERIZING HETEROGENEOUS ELASTIC PROPERTY DISTRIBUTION OF SOFT TISSUES BASED ON AN EXPLICIT INVERSE METHOD

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ABSTRACT

Characterizing heterogeneous material parameters plays an extremely crucial role in the field of biomedical applications. However, classical implicit optimization inverse methods require treating the material parameters of each node or element after the discretization of structural finite elements as optimization variables, leading to a high number of optimization variables. Additionally, for nonlinear constitutive models with multiple material parameters, solving processes can result in an exponential growth of optimization variables. To address these issues, we propose an explicit optimization inverse method based on movable and deformable components. The proposed method only involves optimizing the geometric parameters and material parameters of movable and deformable components, significantly reducing the total number of optimization parameters and improving convergence. The feasibility of the explicit optimization method in reconstructing heterogeneous material fields is validated through numerical comparisons with implicit optimization methods. Furthermore, the explicit optimization method not only provides accurate reconstruction results when using full-field displacement inversion but also achieves precise material distribution when only utilizing boundary displacement measurements. The approach presented herein is expected to effectively enhance the accuracy and efficiency of characterizing the biomechanical properties of soft materials, overcoming the bottleneck issues in performance.

Machine learning for large scale models in physics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE PHYSICS-INFORMED DEEP COMPOSITIONAL OPERATOR

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ABSTRACT

We focus on solving partial differential equations (PDEs) with variable parameters. To this end, neural operators as an effective machine learning method are trained as mapping from these parameters to their corresponding solutions. A significant challenge in training neural operators is the requirement for large datasets of paired input-output examples, which are often expensive and time-consuming to produce. As a solution, neural operators trained through physics-informed methods have gained attention. However, existing physics-informed neural operators struggle with issues such as accommodating irregular domain shapes or generalizing across different dimensions of parameter observations. We propose a novel model architecture that successfully overcomes these hurdles. It is designed to generalize across diverse parameter observation dimensions within irregularly shaped domains. Moreover, this innovative architecture is compatible with physics-informed training, thereby bypassing the need for finite-element methods in creating training data. Our results show that this novel model not only matches but potentially surpasses the performance of traditional data-driven neural operators.

Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A HIGHLY EFFICIENT COMPUTATIONAL APPROACH FOR FAST SCAN-RESOLVED SIMULATIONS OF METAL ADDITIVE MANUFACTURING PROCESSES ON THE SCALE OF REAL PARTS

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ABSTRACT

We present a fast method to simulate metal powder bed fusion additive manufacturing (PBFAM) processes on the part-scale to predict quantities of interest (QOI) such as temperature evolution, microstructural phase composition, and residual stresses. The fundamental computational challenge for part-scale simulations lies not so much in the requirements of the spatial discretization but rather in the large number of time steps necessary to resolve the fast-moving laser path. In contrast to many existing approaches in the literature, our model consistently resolves the physical scan path, enabling new and detailed insights into the scan-strategy-dependent evolution of QOIs, especially for complex geometries.

Starting from a highly efficient thermal model [1], we present an efficient implementation to predict the thermally induced microstructural composition and the residual stress distribution. An emphasis is placed on an implementation that best utilizes available hardware. We use well-established techniques for parallel evaluation on distributed, adaptively refined meshes to distribute the work among available CPUs. Appropriate single instruction multiple data (SIMD) techniques are utilized to speed up the evaluation times significantly. Applying SIMD techniques to constitutive equations and evolution laws requires careful analysis of the different conditional branches within the model equations. All vector accesses and updates are performed in a cache-efficient manner. A performance analysis demonstrates the high degree of optimization of the presented approach. The proposed computational framework allows to perform a coupled thermal microstructure simulation with a consistently resolved laser beam path for the complete build process of the AM Bench 2022 cantilever specimen (312 layers, 30 million spatial degrees of freedom, 50 million time steps) with a time-to-solution below two days. For the coupled thermo-mechanical problem, we present new application-specific solution schemes that enable fast simulations on hundreds of process layers.

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Multiphase flow and non-Newtonian fluid - Modelling and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ANALYSIS OF THE TRANSPORT OF MONOETHYLENE GLYCOL INSIDE OIL PIPELINES USING NUMERICAL SIMULATION AND DEEP LEARNING MODELING

Alessandro Antunes[1], Nathalia Melo[1], João Ferreira Neto[1], Paulo Lyra[1], Jonathan Teixeira[2], Giselle Silva[3] and Darlan Carvalho[1]*

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ABSTRACT

One of the challenges faced by oil production systems is the formation of inorganic fouling, which is one of the problems of flow assurance, caused by the precipitation and deposition of substances such as barium and strontium sulfate, silicon sediments, calcium carbonate and sulfate, iron, and other insoluble solids, in a single phase or combination of different minerals. Effective methodologies are being sought to mitigate or prevent the damage caused by this phenomenon, such as the injection of inhibitors to prevent the nucleation and growth of fouling crystals. The solvent used by many of these inhibitors is monoethylene glycol (C2H6O2), which is a liquid substance of low toxicity, miscible in polar solvents and relatively non-volatile. For this approach to be effective, it is necessary to understand the behavior of the product used for this purpose inside the pipeline, as incorrect injection can accelerate and promote the recurrence of these formations. Therefore, in the present work, in order to understand the effectiveness of cases of inhibition of this phenomenon, we begin to investigate the behavior of the two-phase, multi-component flow resulting from the injection of monoethylene glycol into a mixture of oil and formation water in an oil production system pipeline, using Ansys Fluent, and through a Deep Learning model, in which the predictions obtained through the numerical simulations were used as a training data set. Using both methods, the distribution of the mass fraction of monoethylene glycol in this system was predicted and the influence of different transport speed profiles of this fluid on the coefficient of variation of this fraction was verified, to predict the uniformity of the resulting mixture between this substance and the formation water. Our preliminary results show that the deep learning approach has produced reasonably accurate results at much lower computational costs than that required to carry out the numerical simulations.

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Modeling, simulation, and AI for ultrasonic NDT and SHM
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A PERFORMANCE ANALYSIS PROCEDURE BASED ON CORRECTED DISPLACEMENTS TO EVALUATE THE SEISMIC RESPONSE OF STEEL 2D FRAMES

Jose Mendoza[*1], Berardi Sensale[1] and Alfredo Canelas[1]*

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ABSTRACT

In the proposed methodology, a load pattern is applied in a non-adaptive fashion to obtain the seismic response of two-dimensional steel moment resisting frames. The proposed methodology is based on the structural dynamics theory and consists of a single run nonlinear analysis. This invariant load pattern is formulated by considering higher mode effects with the use of an effective modal mass contribution factor. Also, part of the proposed procedure, a corrective factor is employed to adjust the displacements obtained from the nonlinear analysis ensuring that the drift values obtained from the corrected displacements are adequate. The procedure allows the analysis of the structural response, i.e, story displacement and story drifts. To evaluate the methodology, three benchmark 2D moment steel frames with 3, 9 and 20 stories are analyzed. Material and geometric non linearities are considered for all the cases. The results are compared with the ones obtained by the Nonlinear time history analysis and the Force adaptive procedure.

New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION DESIGN OF FLOW MACHINE ROTORS FOR ROTATING RESONANCE SUBJECTED TO LOW DENSITY FLOWS

Diego Hayashi Alonso[1], *Renato Picelli*[1], *Julio Meneghini**[1] *and Emilio Carlos Nelli Silva*[1]

[1]*University of São Paulo*

ABSTRACT

Resonance is a phenomenon that can easily bring a fluid flow device to fail, and it also portrays different characteristics under rotational motion. Thus, this is an important aspect to consider in flow machine design, beyond just the fluid flow performance. Until now, only the fluid flow performance has been considered in fluid flow topology optimization, still missing the rotating resonance phenomenon. Thus, this work elaborates a new formulation for fluid flow topology optimization considering rotating resonance, while also taking a low mass density (compressible or incompressible) fluid flow into account. The fluid flow-based design now considers three different aspects: the modal analysis (for resonance), the solid structure (for the mechanical behavior) and the low mass density fluid flow (for the fluid flow performance). The topology optimization problem is exemplified for a predominantly radial rotor, which is considered through a simplified 2D model. The different design aspects are considered from a multiobjective function approach. The design variable is nodal, and the optimization algorithm is based on integer linear programming. Some numerical examples are presented for the new topology optimization formulation, showing how the modal and structural effects affect the topology optimization design.

Phase-field models of fracture
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A LENGTH SCALE INSENSITIVE PHASE FIELD MODEL BASED ON IRREVERSIBILITY CONSTRAINT OF FRACTURE PROPAGATION USING LAGRANGE MULTIPLIER

Li Meng[*1], Hsiao Wei Lee[1], Alireza Ashkpour[1] and Ahmad Najafi[1]*

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ABSTRACT

The classical phase field model with second order geometric function α(φ)=φ^2 (i.e., AT2 model), has wide applications in modeling brittle fracture, but nonlinearity and inelasticity are found in its stress-strain curve. The phase field model with linear geometric function α(φ)=φ (i.e., AT1 model), has a linear elastic threshold in its stress-strain curve, which is expected to better model brittle fracture. However, both AT2 and AT1 models are length scale sensitive phase field model, which could have difficulty in adjusting fracture strength and crack band at the same time through a single parameter (length scale). In this study, a generalized quadratic geometric function (linear combination of AT1 and AT2) is used in phase field model, where the extra parameter in this geometric function makes it a length scale insensitive phase field model. Similar to the AT1 model, negative phases can happen in the proposed generalized quadratic geometric function model. To solve this problem in the proposed model, irreversibility constraint of fracture propagation is realized through KKT conditions using Lagrange multiplier, instead of the KKT conditions using strain energy in the classical AT2 model. Several exemplary simulations verify the feasibility of the proposed phase field model, including Mode Ⅰ, Mode Ⅱ, and mixed mode cases. From these simulations, the proposed Lagrange multiplier works well on the irreversibility constraint of fracture propagation. For the proposed length scale insensitive phase field model, it can provide a linear elastic threshold, and a narrower crack band can be obtained, compared to the other two phase field models (i.e., AT1 and AT2).

Computational mechanics in Canada and China: Current states of shared scientific interests and opportunities for the future cooperation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION DESIGN UNDER STIFFNESS, STRENGTH, AND TEMPERATURE CONSTRAINTS OVER A WIDE RANGE OF TEMPERATURES

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ABSTRACT

This article proposes a thermo-elastic topology optimization with stiffness, strength, and temperature constraints involving a wide range of temperatures. The state equations for the linear elasticity and heat conduction are considered. Formulations involving minimum volume with compliance, stress and temperature limits under multiple thermal conditions are presented. The global stress and regional temperature metrics adopting the corrected aggregation function are used to evaluate the maximal stress and temperature, respectively. The stress stabilizing scheme is utilized to overcome the iteration oscillation stemming from highly nonlinear behavior of thermal stress constraints for multiple thermal conditions. To achieve clear optimized topologies under design-dependent loads, a continuation strategy for the relaxed Heaviside function is developed.

Two 2D numerical examples are employed to illustrate the validity and practicability of the proposed approach. The results show that the optimized structures designed by a certain temperature may be damaged or have thermal deformations once the ambient temperature changes due to the thermal residual stress. The designs covering wide temperature range achieved by neglecting stiffness or strength constraints can result in stiffness reduction or strength failure. Optimized topology for multiple heat fluxes works well at different temperatures. Designs with structural and thermal limits have good mechanical performance. Battery pack designed covering a wide range of temperatures validates the method. It is therefore imperative for the optimization to adopt a multi-physics model involving multi-constraints over a wide temperature range.

Contact and interface mechanics: Modeling and computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HOW DOES FRICTION AFFECT SLIDING CONTACT MECHANICS?

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ABSTRACT

Dealing with semi-infinite solids, interfacial friction is usually neglected, as normal and tangential displacements fields are independent on each other (unless material dissimilarity occurs).
However, contacts involving a sufficiently thin layer, do not stick to such a simplified assumption, as thickness related normal/tangential coupling occurs, and surface frictional shear stresses do matter. It is the case, for instance, of classical rotary seals in boundary lubrication regimes, where rough frictional contacts between thin polymeric sealing lips and rotating shafts occur. Also, functional coatings to control the interface (adhesive, frictional, chemical, etc.) behavior, may be very thin and compliant, and usually experience frictional sliding during operation. All the same, these examples indicates that conditions exists where elastic coupling between in plane and out of plane displacements cannot be neglected and must be considered, instead.
Here, we present our results [1-3] on the rough contact mechanics of elastic and viscoelastic thin layers. We assume sliding conditions and Coulomb friction at the interface, and we investigate the contact problem in the framework of linear (visco)elasticity, by relying on the Green's functions approach. We show that, due to the friction and coupling, the presence of interfacial friction may lead to a significant increase of the contact area (up to 10%), compared to the frictionless case, which may affect specific functional response of the interface, such as electrical and thermal conductivity. Since the normal gap distribution is also affected by coupling and friction, the leak rate at the interface turns out significantly altered too. Coupling and friction also affect the contact pressure, which presents a certain degree of asymmetry leading (even for purely elastic materials) to an additional interlocking contribution to the tangential force opposing the relative motion at the interface. Therefore, the overall macroscale friction cannot be predicted by summing-up the local (Coulomb) friction contributions occurring at microscale as commonly expected; it should instead include an additional coupled-induced term. The surface stress tensor is also affected, as due to friction and coupling very high tensile stresses are localized at the contact trailing edge, which are likely to induce material failure.
In conclusion, we show that the common practice to neglect in-plane interactions in contact mechanics may lead to misleading tribological predictions.
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Scientific machine learning for geophysical applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOWARDS TRUSTWORTHY MACHINE LEARNING FOR WEATHER MODELING

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ABSTRACT

In recent years, machine-learning based weather models trained on historical and simulated data have attained an accuracy level that matches or even exceeds those of operational numerical models. Nevertheless, AI-based models are commonly perceived as black boxes, result in compromised credibility in the decision-making process.

This work endeavors to shed light on the reliability of AI-based weather forecast models. First, we introduce dynamical indicators into model evaluation, promoting correct modeling of the underlying dynamics. A comparison of mainstream machine learning and numerical weather models is provided. Second, we implement various post-hoc interpretability methods on GraphCast, fusing the knowledge learned by neural networks and understood by humans. Finally, we inject physical priors into data-driven models leveraging a DeepONet structure.

Multiphysics and data-driven modeling for cardiovascular biomedicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PERSONALIZED AND UNCERTAINTY-AWARE VIRTUAL PLANNING FOR CORONARY ARTERY BYPASS GRAFT SURGERY INFORMED BY CT MYOCARDIAL PERFUSION IMAGING

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ABSTRACT

Coronary artery disease (CAD) is the leading cause of death globally. While coronary artery bypass graft (CABG) surgery improves mortality in patients with severe CAD, long-term outcomes remain a challenge, with 24% of patients reporting chest pain within a year. This is because revascularization is often guided by anatomical risk, which has worse outcomes than treatment based on hemodynamic severity. To address this, personalized computational fluid dynamics (CFD) simulations can improve CAD treatment outcomes via non-invasive hemodynamic risk assessment and virtual treatment planning.

CFD can non-invasively calculate clinically relevant hemodynamics by simulating blood flow in patient-specific anatomies based on non-invasive clinical imaging. However, while current CFD tools are mostly diagnostic, predictive surgical planning requires models that are personalized to the pre-treatment hemodynamics for each patient while linking clinical interventions in large epicardial vessels with downstream flow in myocardial microvasculature. This is a challenge because image-based models are limited to vascular scales that can be resolved by clinical imaging – resulting in models that omit small vasculature and do not reflect true patient-specific coronary flow. Moreover, these models distribute flow amongst arteries empirically, which ignores patient variability and microvascular disease. In addition, while current models are usually deterministic, rigorous uncertainty quantification is crucial for robust clinical translation of such virtual diagnosis and treatment planning tools.

To address these issues, we demonstrate a novel framework for accurate, personalized and uncertainty-aware virtual CABG planning that is informed by clinical data. This framework (1) creates realistic multiscale anatomical models by combining image-based models with synthetic vascular trees to represent arteries that are under-resolved in clinical imaging; (2) estimates personalized model parameters and flow distributions by incorporating patient-specific clinical CT myocardial perfusion imaging and measurements of cardiac function; (3) quantifies uncertainty in model parameters as well as clinically relevant hemodynamic metrics using Bayesian estimation. We show that this framework reproduces patient-specific coronary flow distributions significantly more accurately than the widely-used Murray’s law. Crucially, models personalized to pre-CABG clinical data are able to more accurately predict clinically-measured post-CABG outcomes. This is therefore a promising step towards personalized, multiscale and uncertainty-aware virtual CABG planning.

Contact and interface mechanics: Modeling and computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

OPTIMAL GPU CONTACT IN SIERRA SOLID MECHANICS

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ABSTRACT

Sierra Solid Mechanics (Sierra/SM) is the engineering mechanics simulation code developed at Sandia National Laboratories for modeling highly nonlinear large deformation mechanical events. These mechanical events often involve complex contact solutions. Previously, the Dash contact library, the production contact library in Sierra/SM utilized MPI to efficiently compute contact on CPU dominant architectures. This work extends the contact library to efficiently compute contact on the new GPU dominant architectures of the future.

This presentation will give a brief overview of the Dash contact algorithm in Sierra/SM. We will also look back on the history of porting Dash to the GPU and discuss why these efforts failed to produce satisfactory performance. We will then present the current performance of Dash contact on the GPU, showing the significant speedups realized over current CPU dominant platforms. Details of the contact algorithms used for GPU execution (coarse search, closest-point-projection, etc.) will also be explored. Finally, we will present the future of Dash contact on the GPU and Sierra/SM on the GPU in general.

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IMPROVING ACCURACY, INTERPRETABILITY, AND GENERALIZABILITY OF STRESS INTENSITY FACTOR SOLUTIONS USING SYMBOLIC REGRESSION

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ABSTRACT

Finite element models can be used to obtain high-fidelity stress intensity factors (SIFs), but at the expense of a significant computational cost. In contrast, handbook solutions such as the models developed by Raju and Newman, provide SIF approximations using low-cost surrogate models. A limitation to such handbook solutions is their limited applicability to a set of highly idealized cases. Machine learning offers the ability to produce new handbook solutions for improved accuracy and more complex, practical cases. Genetic programming based symbolic regression (GPSR) adds the ability to maintain the SIF model interpretability that is beneficial to handbook solutions. Interpretable models are desirable due to improved trust. Perhaps equally important is that most engineering software can readily use analytical expressions, like those produced by GPSR, lowering the implementation barrier. In this presentation, we present a direct comparison to the Raju-Newman SIF solution for a semi-elliptical surface crack in a finite plate to models produced using GPSR. Comparisons are made using both accuracy and model complexity as comparative metrics. For GPSR to provide SIF models with acceptable accuracy, a mechanics-based approach (much like the technique used by Raju and Newman) is required in which a known analytical solution is combined (multiplicatively) with geometrical correction functions in a boosting-motivated approach. The GPSR models were found to outperform the Raju-Newman SIF models in terms of accuracy, complexity, and evaluation time.

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Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ACCURACY AND CONVEXITY OF HOMOGENIZED MATERIAL STIFFNESS FOR NON-AFFINE FIBROUS MATERIALS

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ABSTRACT

Fibrous materials are an exceptional class of materials that are found in biological structures ranging from the scale of the cell nucleus to the tissue and organ scales. In the context of collagenous tissues, fiber diameters are typically orders of magnitude smaller than the structures of interest and complex behaviors emerge from the heterogeneous and nonlocal nature of fiber interactions. Capturing this emergent behavior has been a matter of intense interest in the biomedical engineering community spurring many novel continuum scale constitutive relations typically based on an assumption of affine fiber deformations which allows analytical homogenization of the micromechanical response.

Numerous works have shown that fiber kinematics is non-affine for the range of densities and bending lengths typical in biological tissues. And this non-affine behavior, drives the macroscopic behavior. Therefore, multiscale models that can capture the fiber micromechanics, but model problems of biological relevance are needed. To this end, we developed a multiscale finite element code for heterogeneous supercomputers, MuMFiM, that uses computational homogenization of fiber network subscale models, and used these simulations to create machine learned surrogate models. This talk focuses on the computation of the material stiffness as required for the macroscale finite element solve in MuMFiM. Due to factors such as nonlinearity and sub-isostaticity, network structures often have non-invertible Jacobians and are typically solved with explicit or dynamic relaxation methods. This has led to a range of methods for computing material stiffnesses. We will discuss the accuracy, convexity, and range of applicability for four methods as follows: 1) finite differencing of a dynamic relaxation solver [1], 2) machine learned surrogate models using Sobolev minimization to train on energy, stress, and stiffness [2], 3) a specialized non-affine approximation method for fibrous materials described in [3], and 4) and, the classical static condensation method.

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Methods for identification, machine learning, and uncertainty quantification of reduced order models of coupled systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT OF TAILORED FIXTURES AND CONDITIONS FOR 3-AXIS MECHANICAL SHOCK TESTING.

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ABSTRACT

Components of aerospace systems are often subject to pyroshock and other shock loads and, as such, must be qualified for those environments. The most common laboratory setup using an air gun and resonant plate allows for testing in only one direction at a time. However, single axis tests can never perfectly reproduce the environmental loading the component will see in the field. Additionally, large input forces can be required to match certain loads in a single axis which could overload components in an off axis, causing damage or failures to occur. Therefore, it is crucial to design a proper 3-axis test to reproduce the environment as closely as possible. Three-axis tests are complex and tedious to set up to achieve the desired loads.
The first step in using analytical tools for the design of the test fixture is to show that simulation can accurately describe the behavior of the fixture during the test. We have previously developed and validated a fully non-linear finite element model of the airgun resonant plate 3-axis shock test. The model has all important features parametrized, including geometry of the fixture, location of the test object on the fixture, impact point, and dimensions and velocity of the projectile. To develop the fixture and test conditions that result in shock loads that match provided specifications, advanced optimization techniques based on design space exploration, construction of surrogate models using Gaussian Process Models, sensitivity analysis and global optimization both for scalar and functional quantities of interest were used.
The method developed for optimization of test fixture and conditions allowed for the reproduction of 3-axis shock loads in a single laboratory experiment without multiple iterations in hardware, thus not only facilitating qualification of components under more realistic conditions, but also reducing required time and cost.
We will present results of the fixture development for the real-world test and predictions of the designed test performance.
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ON THE TRANSIENT BEHAVIOR OF ROTOR-STRUCTURE-FOUNDATION-SOIL SYSTEMS

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ABSTRACT

The modelling of the transient dynamic response of rotor-structure-soil systems is important in many situations such as blade failure in the wind turbines, sudden electrical load changes in the wind turbine generator and incoming wave fields hitting the foundation due to earthquakes or blasts. The modelling and solution of the transient behavior of these coupled systems is a challenge due to the dynamics of the rotating system but also because of the soil response presenting geometric damping.

The frequency domain response of a Laval (Jeffcott) rotor interacting with a rigid foundation on an elastic half-space was presented by Maurer et ali. [1]. An extension of this work to include more complex and realistic viscoelastic and layered soil models was presented by Carrion et ali. [2].
In the present work a methodology is introduced that allows to model the transient response of a Laval rotor interacting with a frame structure supported by a foundation interacting with a soil profile. The system is subdivided into two sub-systems. In the first subsystem, the transient dynamic response of the structure-foundation-soil is obtained by a modified modal analysis procedure [Amauri, 3]. For the second subsystem, the governing equations of the Laval rotor with damping mechanisms are integrated in the time domain. The dynamic coupling of both subsystem by a numerical dynamic coupling scheme allows the determination of the transient behavior of the coupled RSFS system.

In the numerical examples, the role of the internal and external rotor damping mechanisms and the soil geometric damping are analyzed in a rotor run-up passing through its resonances.

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EFFICIENT RANDOMIZED ITERATIVE SOLVERS FOR UNSYMMETRICAL PROBLEMS IN COMPUTATIONAL MECHANICS

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ABSTRACT

Solving large-scale linear systems resulting from partial differential equations poses significant challenges in both computation and memory storage. This difficulty, however, creates opportunities to reconsider traditional numerical algorithms within the context of extensive data and massively parallel supercomputers [1]. In the last decade, a novel approach has emerged, leveraging randomization to accelerate linear algebra operations [2]. This method demonstrates impressive efficiency, achieving linear complexity O(N) with respect to problem size, as validated in various dense linear systems, including integral equations, statistics, and machine learning.
In contrast to our previous work [1,3] focused on dense and low-rank systems, this presentation explores the possibilities and hurdles of applying the randomization approach to intricate systems originating from Fluid and Solid Mechanics problems. These systems are characterized by sparsity and frequent ill-conditioning. The emphasis will be on incorporating appropriate sketching techniques into the construction of the Krylov method to enhance the performance of the underlying iterative solver. The talk will include the presentation of 2D and 3D applications to evaluate the efficacy of this new paradigm.

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Data-driven methods for modeling complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RECENT ADVANCES IN WEAK-FORM EQUATION LEARNING WITH APPLICATIONS TO MULTISCALE PHENOMENA

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ABSTRACT

Equation learning has arisen as a paradigm for constructing governing equations for phenomena of interest using observations of the underlying system. In the context of differential equations, a consensus has formed that weak-form equation learning (WFEL) offers many advantages, such as implicit noise filtering, high accuracy, and reduced regularity requirements on the ground-truth data. In this talk I will review essential components and theoretical results of the WSINDy algorithm (Weak-form Sparse Identification of Nonlinear Dynamics) to demonstrate these advantages in the discovery of ordinary and partial differential equations. I will also delve into a new paradigm for which WFEL appears to be particularly well-suited, that of inference for multiscale systems. Recent works have shown that WSINDy can aid in the discovery of interpretable mean-field laws for large systems of particles, homogenization of highly-oscillatory media, and coarse-graining of Hamiltonian systems with approximate symmetries. I will survey these results and with applications to cell migration experiments, and provide a general outlook for this line of research.

Computational mechanics for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ACTIVE LEARNING TO ACCELERATE THE QUALIFICATION OF ADVANCED MATERIALS FOR HARSH CONDITIONS

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ABSTRACT

Under harsh conditions material properties are seldom static as the environment alters the material chemistry and microstructure over time. Qualifying materials for service in harsh conditions therefore often requires developing and fitting a model to predict how the material properties will change under the expected service conditions. Calibrating and validating these models usually requires some amount of long term testing in representative environmental conditions. Extensive long-term testing greatly slows the qualification of new materials, as, by definition, these tests have long durations and often require expensive test setups to replicate the target service environments. Traditionally, simple gridding approaches have been used to select particular test conditions within target windows and the maximum duration of tests have been selected with rules derived from engineering experience. This talk describes the potential in replacing these traditional methods with active learning approaches. Specifically, the talk focus on using active learning to select creep test conditions, with the goal of developing an accurate model for long-term creep behavior. Several active learning strategies are compared to gridding test conditions or selecting conditions randomly, in order to quantify the advantages of active learning in reducing the number of tests required to reach a desired level of accuracy.

Advanced simulation techniques for the structural design of carbon reinforced concrete
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A HOMOGENIZATION APPROACH FOR THE ANALYSIS OF SHELL STRUCTURES EMPLOYING IMAGE-BASED METHODS

Leonie Mester[*1], Simon Klarmann[1] and Sven Klinkel[1]*

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ABSTRACT

In the field of civil engineering, the enhanced corrosion resistance offered by textile reinforcement allows for the construction of slender structures. Nonetheless, the complex internal structure makes a detailed analysis challenging and computationally expensive. To address this issue, a multiscale method for the efficient structural analysis of shell structures is proposed. The structural problem is investigated at two scales: a macroscopic scale that describes the shell structure and a mesoscopic scale that describes the material response. The inherent global periodicity found in biaxial grid-aligned textile reinforcement, which is commonly used in civil engineering, facilitates the definition of a representative volume element (RVE). The RVE describes the characteristic geometric and material properties of the mesostructure. A volumetric representation is employed, allowing a detailed investigation of the mesoscopic constituents, namely the textile reinforcement and the surrounding matrix. Structural shell elements are used for analysis at the macroscopic scale, reducing the volumetric problem to a two-dimensional problem. This dimensional reduction simplifies the geometry. However, the reduced dimension, namely the thickness of the shell, is considered by the RVE, since a distinctive feature of the presented approach is that the height of the RVE corresponds to the macroscopic shell thickness. The presented multiscale method is a first-order homogenization approach governed by the Hill-Mandel condition. The focus is on the choice of appropriate boundary conditions for the RVE to ensure a consistent coupling between the macroscopic structural shell element and the mesoscopic volumetric description of the RVE. To enhance the accuracy of the geometric description of the textile reinforcement, image-based methods are combined with scaled boundary isogeometric analysis (SBIGA) at the mesoscopic scale. A parameterized RVE is presented, which considers the characteristic geometric properties of the textile reinforcement. Linear-elastic benchmark examples demonstrate the validity of the proposed approach. The homogenized stiffness components exhibit an erroneous dependence on the in-plane RVE size, which is effectively addressed by introducing an internal constraint. To show the suitability of the parameterized RVE using image-based methods, experimental data from carbon-reinforced concrete shell specimens is used. Finally, a simulation of a textile reinforced concrete specimen incorporating the nonlinear material behavior demonstrates the applicability of the present homogenization approach.

Multiphysics and data-driven modeling for cardiovascular biomedicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NEURAL-NETWORK FINITE ELEMENT APPROACH FOR SIMULATING TRILEAFLET HEART VALVES WITH FULL MULTI-BODY CONTACT

Kenneth Meyer[*1], Christian Goodbrake[1], Shruti Motiwale[1] and Michael Sacks[1]*

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ABSTRACT

Due to the inherent pathophysiological complexities of heart valve disease, computational modeling in directing patient-specific therapies has great potential to provide accurate predictions and determine optimal treatments. The Finite Element Method (FEM) solves the partial differential equations governing heart valve closure with high accuracy, but remains too slow to implement in clinically relevant timeframes. To simulate heart valve closure in clinically relevant timeframes, we adopted our Neural-Network Finite Element (NNFE) approach. Previous NNFE-related work has shown a Neural Network can capture the deformation of a flat plate under a pressure load without loss of accuracy when compared to FEM simulations [1]. To clarify, the NNFE approach is not data-driven, but rather it uses NN as universal function approximator of the displacement field, with training driven by minimizing the gradient of the potential energy of the system. Finite Elements are still used to discretize the physical domain, apply boundary conditions, and perform necessary numerical integrations. Recent developments have shown the NNFE approach can simulate contact of an elastic body using a frictionless symmetry plane [2].

This work extends upon these studies to incorporate full multi-body contact into the NNFE approach to simulate a trileaflet heart valve in a generalized manner. The energy penalty term used to enforce contact in [2] was modified to compute the distance between each leaflet pair to check for penetration. The NN displacement field was then trained over the physiologically admissible range of pressures a valve experiences during closure. Once trained (12hr), it takes the NNFE model only 5.34s to compute displacements on a NURBS mesh with 147 control points and 5.75s with 720 control points, while the traditional FEniCS solutions take 89.36s and 788.53s for the same problem sizes, respectively. Thus, as in our previous studies the scaling of problem size produced results without increased solve times when simulating full multi-body contact. To the authors knowledge, this is the first demonstration of full multi-body contact using NN methods. This work advances the capabilities of Machine Learning in cardiovascular modeling and simulation.

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Data-driven modeling and design of materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMBINING PENN, EQUATION DISCOVERY, AND NOVEL PLASTICITY FRAMEWORKS

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ABSTRACT

When using neural networks as components in plasticity model evolution laws, it is possible to enforce physics directly [1]. These Physics Enforced Neural Networks (PENN) models intrinsically fulfill, e.g., the dissipation inequality and frame invariance. Such strong enforcement of physics has been shown to generalize better than penalty enforcement [2]. Consequently, PENN-based plasticity models hold promise for accurate and reliable predictions of material behavior. Another advantage lies in the flexible incorporation of desired model assumptions, such as isotropy and pressure-independent yielding, thereby reducing the required training data size. However, when enforcing such restrictions, it is paramount to not exclude relevant processes. One such restriction is the definition of a yield surface separating distinct elastic and plastic regions. As macroscopic constitutive models represent the homogenized behavior of a heterogeneous microstructure they must also consider how different parts will yield at different load levels resulting in a smooth elastic to plastic transition. A novel plasticity framework, denoted the "Degree of Plasticity" model, addressing this challenge is combined with PENN evolution laws in this contribution. Furthermore, using the equation discovery from [1], we identify analytical evolution laws from the trained neural network, resulting in an interpretable and efficient constitutive model discovered from data.

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Data-driven modeling and design of materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SEQUENTIAL DESIGN OF PLATE-LATTICES

Paul Philipp Meyer[1], Thomas Tancogne-Dejean[1] and Dirk Mohr[1]*

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ABSTRACT

Periodic architected materials, characterized by their fundamental building blocks as truss-, shell-, and plate-lattices, have garnered significant attention in material science and engineering. The elastic response of plate-lattices with cubic symmetry reaches theoretical limits for isotropic response, exhibiting optimal mass-specific stiffness. We believe the potential of plate-lattices extends beyond isotropic structures. The primary objective is the strategic development of stiff lattices with tailored properties. This study introduces a general construction method of plate lattices, defined as an assembly of plates and intersections. It involves sequentially placing plates within the unit cell, with the choice of an anchor point, a normal vector, and a thickness, under the constraint of periodic conditions. Building upon this general formulation, a large-scale comparison to the property spaces of truss- and shell-lattices is presented. We demonstrate that versatile arrangement of plates offers geometry control over a large macroscopic property space for the same constituent material. Furthermore, we describe a correlation between plate orientation and stiffness. To tailor the lattice properties, we utilize a recurrent neural network designed for the inverse question—mapping from property to structure. Our findings reveal the efficacy of the inverse model in generating lattices with targeted properties. Three illustrative cases, including the hexagonal honeycomb, SC plate-lattices, and SC-FCC plate-lattice, highlight the model's capacity to extrapolate lattice designs beyond training data parameters. We further demonstrate the model's ability to unveil the inherent invariance of stiffness to the plate position. In conclusion, this research not only advances the understanding of plate-lattice formulations but also introduces a groundbreaking approach to plate-lattice design through neural network-driven methodologies.

Data-driven approaches for solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREDICTION OF FORMING PROCESSES UNDER UNCERTAINTY

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ABSTRACT

Sheet metal forming is a widely employed manufacturing process that enables the creation of intricate shapes and structures using flat metal sheets, which would be impractical or unfeasible with other manufacturing methods. The change in shape of the sheet metal directly affects the final product's quality, performance, and integrity. The design of forming processes (constrained to a targeted shape) poses a significant challenge due to the complex interplay of vast material, geometric, and other process parameters. The interplay of these parameters can give rise to several complicated phenomena. Wrinkling, for instance, manifests as unintended buckling or folding of the metal sheet, resulting in an uneven surface, typically near the sheet's edges or at the cup's bottom. Here, we propose to eliminate such uncertainties in the design of forming processes by analyzing a substantial portion of the design space efficiently. We provide evidence of the effectiveness of Convolutional Neural Networks (CNN) in accurately predicting the final shape of elastoplastic metal sheets during forming processes. We differentiate between two cases: the prediction of the forming process with fully known and partially unknown parameters. For the first case, our CNN achieves remarkable accuracy, with a Mean Relative Error below 0.1% when predicting the thickness distribution for previously unseen parameters. We analyze the model's performance dependence on factors such as model size, training process, and available training data. We emphasize the capability of neural networks to accurately predict nonlinear wrinkling of the sheet. For the second case, we develop an attention-based diffusion model mapping partial parameter sets of the forming process to the probability distributions of resulting shape. We find matching distributions between the predictions and the uniformly random sampled testing data. We leverage this capability to quantify the uncertainty resulting from unknown friction during forming processes. We obtain spatial uncertainty estimates, enabling the designers to judge the manufacturability and improve the process robustness efficiently.

Architected materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RETHINKING TOUGHNESS: USING NANOSTRUCTURE TO ENHANCE THE DURABILITY OF ADDITIVELY MANUFACTURED MATERIALS

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ABSTRACT

Strength and toughness are both highly desirable properties of structural materials, but they are often considered mutually exclusive. Much work has gone toward developing materials that are both strong and tough using different composite architectures and material processing techniques, but they generally ignore the role of length scale and structural size-effects on toughness. In this work, we develop nanoarchitected polymeric materials that utilize both heterogeneity and size-affected ductility to enhance their toughness without sacrificing strength. We create specimens with layered architectures in a micro-single edge notch bend configuration using two-photon lithography and various post-processing techniques. Gradually reducing the layer thickness (D) resulted in an increased fracture energy and slower, stable crack propagation, a phenomenon that became pronounced as the layer thickness approached or was smaller than the material fracture process zone (D ≦ FPZ). The thinnest of these layered structures demonstrated an increase in toughness by 5x from 60 J/m2 to 300 J/m2 as interlayer spacing was increased from 0 to 4 um, a value that is augmented by the creation of heterogeneity along the crack path. Notably, these materials do not show an appreciable loss in strength or stiffness up to an intermediate layer spacing despite a ~40% reduction in density. The results of this study not only demonstrate the large degree of tunability in these architectures but also show how to fundamentally utilize size effects to create architected materials with unprecedented properties.

Modeling and learning of structured dynamical systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ESTIMATION OF DEPLOYMENT DYNAMICS OF A TAPE-SPRING BOOM USING RATIONAL LEAST-SQUARES FITTING

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ABSTRACT

The need for composite booms in deployable space structures is ever-increasing. This effort studies the effects of environmental conditions on the material properties of a self-deployable carbon fiber boom with a parabolic cross-section. The deployment velocity and the internal strain energy of this boom are highly sensitive to temperature changes. The same boom will fly as the primary payload on Ut ProSat-1 (UPS-1), a 3U CubeSat designed and manufactured by students at Virginia Tech. The boom will be deployed repeatedly across the full range of spacecraft's environmental conditions. In addition, the boom has a flexible circuit near its tip. This circuit houses an inertial measurement unit (IMU) to measure the acceleration experienced by the boom during and at the end of each deployment sequence. A second IMU embedded on the payload control module near the root of the boom measures the base vibration response. The on-orbit data will validate the model obtained from the ground experiments described here. The boom was deployed inside a Tenney environmental chamber to simulate the space environment. The thermal cycling went from 4°C to 70°C and had dwell periods at each. A low vacuum pressure of 9 Torr was maintained throughout the test.

Characterization of the satellite payload parameters is necessary to validate these results and understand the effects of temperature changes on the deployments. Transfer functions were obtained from the two IMUs and then interpolated to form a low dimensional numerical model by minimizing the least square errors through the process of rational least-squares fitting via vector fitting (VF). While the ideal boom has a constant parabolic cross section, the deployed boom has a variable cross section due to its boundary conditions and small manufacturing defects. The 4-ft (~1.2 m) long boom was measured at 5 cm intervals, starting from the root to the tip, to create a continuous boom CAD model from these profiles. The modal analysis of the boom was obtained using a shell-based finite element (FE) model and the global mass, stiffness and damping matrices were extracted. These are used to obtain the state matrices of the system which are then compared to those obtained via the VF approach. Therefore, the FE model is used to validate the rational approximation procedure. These results will provide insight into the characterization of NASA's tape springs and aid in making informed decisions for future missions while enabling a validated temperature dependent model.

HOW DOES OFF-FAULT PLASTICITY CONTROL FAULT ZONE SEISMOGENESIS?

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ABSTRACT

Professor Selvadurai's foundational contributions in understanding the mechanics and physics of coupled processes in a variety of systems have inspired many works in biomechanics and geophysics including ours. Here, we investigate a long-standing challenge in geophysics related to genesis of fault zones and its connection to observed seismicity. We simulate the co-evolution of shear fractures on pre-existing fault surfaces and bulk inelastic deformation through modeling a sequence of (fast) earthquakes and (slow) aseismic slip of a 2D rate-and-state frictional interface embedded in a full-space elastic-plastic bulk. We use a computationally efficient hybrid finite element spectral boundary integral (FEBE) scheme that relies on domain decomposition in space and extreme adaptive stepping in time. The hybrid computational scheme enables exact near-field truncation of the elastodynamic field allowing us to use high resolution finite element discretization in a narrow region surrounding the fault zone that encompasses the potential plastic deformation. Wave propagation and long range static stress transfer in the exterior half spaces are handled using the spectral boundary integral equation. The adaptive time stepping is based on the maximum velocity jump across the fault surface. The resulting time step varies from milliseconds to days enabling the simulation of both slow deformation and fast dynamic ruptures over multiple earthquake cycles.

Our study reveals that off-fault plasticity can cause both partial ruptures and temporally clustered seismic activities as well as partitioning of permanent deformation between the fault and the bulk. If the yield stress is high relative to the fault’s frictional strength, the plastic deformation dissipates only a few percent of the total energy budget. Nonetheless the impact of plasticity in this case on the seismic cycle can still be significant through its effect on stress distribution and viscous relaxation. Conversely, if the bulk yield stress is low enough to be comparable to the fault's frictional strength, new rupture patterns emerge. These are marked by extensive energy dissipation within the bulk and slow or creeping ruptures on the fault without much noticeable inertia effects. Considering a Weibull distribution of yield strength, the long-term seismic pattern turns out to be governed by the average yield strength rather than its spatial variability. Our findings highlight the pivotal role of bulk strength in earthquake dynamics across different scales and propose a novel aspect of dynamic variability in earthquake physics, potentially influencing earthquake size and energy distribution.

Fluid-structure interaction in interface and moving boundary problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HIGH-ORDER SIMULATIONS FOR FLUID-SOFT SUBSTRATE INTERACTION THROUGH EULER-LAGRANGE AND EULER-EULER FRAMEWORKS

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ABSTRACT

Our research introduces an advanced extended discontinuous Galerkin method (XDG) tailored for the accurate simulation of multiphase scenarios, specifically addressing challenges associated with three-phase contact lines on deformable solids. Singularities at interfaces and contact lines, characterized by abrupt pressure and surface tension changes, present difficulties for high-order methods that traditionally rely on smooth functions for optimal convergence.

Our investigation focuses on simulating a water droplet on a surface made of silicone gel. This simulation incorporates Navier slip boundary conditions at the interface and Young's equation at the three-phase contact line. To provide a comprehensive analysis, we leverage both the Euler-Lagrange and Euler-Euler frameworks. This dual-framework approach enables us to capture the intricacies of the simulation from two distinct yet complementary perspectives.

In our forthcoming presentation, we will conduct an extensive comparison between the Euler-Lagrange and Euler-Euler models, featuring three-dimensional simulation results. Through the presentation of these results, we aim to provide valuable insights into the strengths and limitations of each model. This detailed analysis is designed to contribute to a deeper understanding of these frameworks in the context of simulating complex multiphase phenomena.

Multi-scale modeling and upscaling for flow induced vibrations, from local reference simulations to certified industrial tools
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RANS AND LES SIMULATIONS OF FLOW-INDUCED VIBRATIONS IN ROD BUNDLES WITH MIXING GRIDS

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ABSTRACT

Flow-induced vibrations (FIV) are an important phenomenon to maintain operational conditions in existing nuclear power plants and for future designs. Vibrations arise due to the load induced by the fluid flow on long and slender rods in the core, steam generator and heat exchangers. Their effect can range from fretting to fatigue and may induce early wear or even failure of the mechanical components.
As part of the research effort conducted by the CEA on FIV, an Arbitrary Lagrange-Euler (ALE) method has been implemented in TrioCFD [1] to study fluid-structure interaction. This tool has been successfully employed to reproduce analytical results in state-of-the-art configurations [2], but its capability to predict the vibrations in a realistic setup has yet to be determined. In the present study, as part of the European GO-Viking project, numerical simulations are undertaken to assess the ability of TrioCFD to reproduce the FIV measurements performed on ALAIN experiment [3]. The investigated setup is made of a 5x5 rod bundle with a split-type mixing grid encased in a square duct in which water flows axially at Re=90 000, mimicking the core of a pressurized water reactor.
The ALE method is employed to account for the influence of the fuel-rod assembly moving boundaries on the turbulent flow. Comparison between the numerically predicted FIV and the experimental measurements is conducted for two classes of flow modelling approaches. One, in which the mean flow is determined by solving Reynolds Averaged Navier-Stokes equations (RANS), is commonly employed in industry. The second involves solving filtered Navier-Stokes equations to capture the largest eddies of the turbulent flow (LES) and includes a higher level of detail of the flow features. Analysis of the results provides insight into the capacity of the ALE module of TrioCFD to reproduce experimental FIV measurements, and allows to propose guidelines for FIV simulations in an industrial context.

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Machine learning for large scale models in physics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEEP REINFORCEMENT LEARNING-BASED FLOW OPTIMIZATION FOR IMPROVED WIND RESILIENCE OF SOLAR PANEL ARRAYS

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ABSTRACT

Among the renewable energy solutions of today, solar - more specifically photovoltaic (PV) - power plants are seen as key actors of the energy transition in Europe, and are taking on new designs and functions, seeking more adaptability and efficiency. However, PV power plants still face the major risk of strong winds often leading to breakage, hindering the efforts of green energy development. The aerodynamic loading of PV panels in wind flow has become an important research topic to quantify breakage risk and limits, but such approaches in the literature have been limited so far to panel spacing and simple tilt configurations. We introduce here a novel approach combining high-fidelity numerical simulations of large scale PV fields subjected to a turbulent atmostpheric boundary layer wind flow, and a Deep Reinforcement Learning (DRL) algorithm trained to optimize the individual tilts for the purpose of maintaining safe aerodynamic efforts. An efficient and flexible computational pipeline has been developed, in which the mesh is adapted anisotropically around the fluid-solid interface using a metric map built after simulation-dependent parameters based on the boundary layer theory. The wind flow is computed with an in-house variational multiscale (VMS) stabilized finite element solver. The latter can be applied efficiently to high Reynolds number flows (since the built-in small-scale component of the solution operates as an implicit large eddy simulation) and supports elements of aspect ratio up to the order of 1000:1, which is key to solve the numerically complex strongly anisotropic wind motion generated by the extremely thin build of the panels. Finally, DRL optimization is achieved with the in-house single-step PBO algorithm, that interacts once per episode with the environment to learn the mapping from a given initial state to the optimal action, and uses heuristics from the CMA-ES evolution strategy to exploit the anisotropy of the cost function in the descent direction. The main sub-processes of PV field simulations are seamlessly integrated within a single agent-environment workflow. This includes the geometric computational domain creation from an array of panel tilts, the mesh adaptation algorithm, CFD simulations, and reward computation. We will discuss results obtained for 2d and 3d arrangements of 6 full-scale panels mounted on stands, whose individual tilts are optimized under various reward functions and using different turbulence models. Each optimal configuration is non-intuitive and reward-specific, and will be shown to perform better than the classic tilt configurations found in the literature.

Advances in computational biomechanics and mechanobiology
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ASSESSMENT OF CARTILAGE STIFFNESS HETEROGENEITY VIA ELASTOGRAPHY IN POST-TRAUMATIC OSTEOARTHRITIS

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ABSTRACT

Healthy articular cartilage is comprised of a layered architecture, characterized by superficial, middle, and deep zones, with each zone's components differing in biochemical and mechanical properties and critical for the maintenance of cartilage function. Osteoarthritis (OA) disrupts the zonal architecture of cartilage, where proteoglycan loss leads to loss of mechanical function (eg, decreased compressive strength) [1]. Noninvasive imaging techniques such as elastography show potential to quantify material stiffness and provide a powerful approach to understanding structure-function relationships in load-bearing tissues, specifically in cartilage. Elastography is any imaging approach that is commonly used to quantify the average and spatially resolved stiffness of soft tissues. In cartilage, softening and decreased stiffness in the superficial zone is a functional hallmark of osteoarthritis (OA) pathogenesis due to structural changes to the collagen network and depletion of proteoglycans. As proteoglycans are a primary determinant of stiffness in articular cartilage, the ability to spatially map local stiffness changes within articular cartilage presents a direct link between structural cartilage changes and stiffness, and an opportunity to diagnose early OA via noninvasive imaging.

Recently, our group developed a biomechanically based elastography imaging method that utilizes spiral displacement encoded stimulated echo MRI (spiral DENSE) displacement data as an input [2, 3]. In this work, we used forward finite element (FE) simulations of cartilage-like geometrical shapes and material properties to validate the method, resulting in an average voxel-wise error of less than five percent. We then utilized spiral DENSE displacement data to quantify relative modulus of femoral cartilage in human participants [2]. Other work within our group has established spatial gradients indices of structural (relaxometric) MRI as a method that can evaluate structural and functional heterogeneity through the cartilage depth as a sensitive biomarker of early OA [1]. In this work, we collected spiral DENSE MRI data on 35 patients at approximately 6 months post ACL surgery, as well as an age, sex and BMI matched control cohort. We used the DENSE MRI displacement data as input to our elastography pipeline to calculate maps of spatial modulus within the cartilage. We then calculated spatial gradient indices, defined here as the through-thickness spatial gradient for the modulus, to assess cartilage stiffness heterogeneity [3]. We expect that through-thickness moduli gradients will be more uniform in the control cohort compared to the joint-injury cohort.
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Coupled computational mechanics: Solutions for FSI simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODIFIED IMMERSED FINITE ELEMENT METHOD (MIFEM) FOR EXPLICIT EULERIAN TO EXPLICIT LAGRANGIAN COUPLING

Scott Miller[*1], Anthony Agelastos[1], Mark Christon[1], David Hensinger[1], Chad Hovey[1], Matthew Mosby[1], Jennifer Rees[1], Jesse Thomas[1], Benjamin Treweek[1] and Michael Wong[1]*

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ABSTRACT

The modified Immersed Finite Element Method (mIFEM) [1] is an overlapping mesh method that couples a Lagrangian foreground solution with an Eulerian background solution. We explore using the mIFEM to couple two production codes: an explicit Lagrangian solid mechanics code (Sierra Solid Mechanics) and an explicit, Eulerian (Lagrange step plus remap step), finite element, multimaterial shock physics code (SABLE). Temporal accuracy and stability are essential for the blast-on-structure and impact/penetration classes of problems for which the coupling is designed. We present the details of the mIFEM coupling method and numerically investigate the accuracy and stability properties on a set of exemplar problems. Finally, the fully parallelized implementation is demonstrated with a full scale example problem.

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Current trends and advances in enriched finite element methods and coupled simulations
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TEMPORAL ANALYSIS OF THE GENERALIZED FINITE ELEMENT METHOD FOR MULTI-SCALE HEAT TRANSFER PROBLEMS

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ABSTRACT

The extreme thermal environments encountered by high-speed flight vehicles dominate the design process. The appearance of impinging shock waves and complex shock interactions create sharp, localized thermal gradients that challenge numerical simulations. These challenges are amplified when non-stationary gradients are present due to translating shocks. The combination of these issues leads to standard methods producing accurate solutions inefficiently and at a large computational expense since broadened regions of fine-scale resolutions are required. Thus, there is growing interest in developing methods capable of producing high-fidelity solutions to multi-scale problems at a reduced cost via coarser meshes and less degrees of freedom. The generalized finite element method (GFEM) offers the potential to achieve this goal by modifying the FEM framework for the inclusion of solution-tailored functions into the computational domain and aid in approximating fine-scale features. Therefore, I hypothesize that GFEM can lead to time-accurate solutions at a reduced computational cost compared to standard methods.

The temporal behavior of the GFEM is studied under a model problem exhibiting localized, sharp, and translating gradients. The GFEM framework is leveraged to build global-local enrichments tailored to localized features within the problem domain. The results presented will compare the temporal accuracy, convergence, and computational cost of the global-local GFEM (GFEMgl) and polynomial-enriched GFEM applied to the model problem with the generalized alpha-method as the time integrator. Demonstrative results reveal the solution-tailored enrichments achieve high-order solutions at a significant reduction in computational cost while retaining the expected convergence criterion compared to polynomial enrichment bases. The GFEMgl can resolve fine-scale features on significantly coarser meshes and less degrees of freedom. The temporal robustness of the GFEMgl will be demonstrated through parametric studies to show the method's predictable behavior for various situations. Results will highlight that temporal convergence and accuracy can be safely predicted. The culmination of the results obtained will signify the GFEM’s capability as a high-order numerical method granting high-fidelity solutions efficiently and inexpensively.

Computational modeling of extreme-loading events
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTATIONAL MODELING OF CATEGORY 5 HURRICANE LOADING EVENTS ON A COMPLEX STRUCTURE

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ABSTRACT

Often when hurricanes make landfall, they destroy civil and electrical infrastructure leaving communities without critical infrastructure for long periods. As climate change is causing hurricanes to increase in frequency and forcefulness, designing in coastal areas must consider hurricane resilience. This research has determined the resilience and robustness of an architecturally unique and geometrically complex structure designed for electrical and civil infrastructural applications when subjected to category 5 (CAT 5) hurricane conditions. A history of hurricanes impacting The Bahamas and how their characteristics can be modeled is briefly reviewed. Computational fluid dynamics (CFD) is used to characterize the loads (shear stress and pressure loading) induced by a CAT 5 hurricane on the structure. The CFD software used in this research is OpenFOAM®. The mean wind direction of the hurricane relative to the structure that causes the most severe loading was tested and determined. Both steady and unsteady CFD methods were used to identify the magnitude of loading. Both wind and storm surge loading conditions are considered in the analysis. The wind conditions were modelled using the upper limit of possible CAT 5 wind profiles. The storm surge conditions were modelled after the infamous storm surge profile caused by the 2019 tropical cyclone, Hurricane Dorian, as it passed over The Bahamas. The structural response of the structure under the identified loads found is evaluated via an uncoupled finite element analysis (FEA) approach. The FEA solver Abaqus® was applied to test the complex structure’s robustness and resilience to severe hurricane loading. The two materials considered in the FEA model were a proprietary composite material specifically designed for this application and 1080 steel. The results of the two materials were then compared. Considering the scope and limitations of the research, more work is needed to better understand how resilient the structure is to impact wave loading. The work presented will show that it is possible to design geometrically complex structures and accurately model them using computer aided engineering (CAE) for resiliency to natural disasters.

Recent advances in computational fracture mechanics and failure analysis
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A FAST METHOD FOR COMPUTING ARBITRARY-ORDER STRESS INTENSITY FACTOR DERIVATIVES OF 3D FINITE ELEMENT SIMULATIONS USING HYPERCOMPLEX AUTOMATIC DIFFERENTIATION

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ABSTRACT

This work presents a novel approach to efficiently compute arbitrary-order derivatives of Stress Intensity Factors (SIF) from Finite Element analyses. The method can compute SIF derivatives with respect to any design parameters like material, loading, and geometrical properties (e.g. crack length). The method consists of three steps: first, conventional software is used to compute the displacements of the finite element problem. Second, the stiffness matrix of the conventional problem is computed in a separate module. Finally, Hypercomplex Automatic Differentiation (HYPAD) is used on the residual form of the problem to form systems of equations that solve the derivatives of the displacements with respect to each parameter of interest. The displacements and its derivatives are used in hypercomplex form on the Interaction Integral calculations to compute the stress intensity factor and its derivatives. Preliminary case studies on a flat and inclined penny-shaped crack 3D simulations show that derivatives up to third order with respect to 4 parameters (34 derivatives in total) were computed within the equivalent time of an additional finite element simulation. Derivatives show excellent agreement with the corresponding analytical solutions, with errors within the same order of magnitude as the original displacement solution error. Derivatives of the SIF can be used to generate reduced order models of the SIF, uncertainty analysis, advance the crack front, optimization, and inverse problems.

Honoring the Legacy of Prof. Patrick Selvadurai
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MECHANISTIC COMPUTATIONAL FRAMEWORK FOR SIMULATING A PANDEMIC AND SOCIAL RESPONSE IN A HETEROGENEOUS POPULATION

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ABSTRACT

The COVID-19 pandemic of 2020 has been of epic proportions that has led to a surge in the modelling and simulation of infectious diseases. The paper develops a new model that uses a mechanistic approach to describe interactions between discrete entities (agents) driven by social, cultural, epidemiological, and virological rules in a disease infected population. This ‘granular’ view is borrowed from geomechanics of granular media where large-scale systems such as sand masses derive their behaviour and strength from the mutual interactions between particles through simple force contact laws. Specifically, the proposed computational framework is multiscale starting from the virological-immune system interaction at the scale of an individual to transmission of the virus at the individual-to-individual scale according to rule-driven interactions that are non-probabilistic in contrast to other approaches. As such, the dynamics of the various multi-scale processes of naturally upscale in a nonlinear fashion to larger population sizes with new properties just like in complex systems.

The starting point is a population of discrete particles (individuals) that is initially uninfected—then infections are seeded in the population. Contracting an infection depends on characteristics of each individual—age, underlying conditions, and socio-economic status as well as the viral transmission which is linked to the viral load carried by each infected individual. At the individual (local scale) level, the biological processes are mathematically described through a Lotka-Volterra set of two ordinary non-linear differential equations to describe a predator-prey mechanism where viral growth rate is antagonized by the activation of the immune system.

Mobility of individuals within the population is computed within a discrete element approach driven by social policies such as public health restrictions and workplace protocols. The global population is allowed to evolve over both time and space to lead to the emergence of structures of Susceptible-Infected-Recovered (SIR) type populations using non-phenomenological data. The model is non-probabilistic with the important feature that the viral load evolves for everyone in a population so that at any one time, individuals may be at different deterministic positions within their personal viral load timeline. Airborne aspect of virus propagation can also be incorporated in the model such as the distribution and location of tiny droplets (aerosols) produced by a cough using computational fluid dynamics. Numerical examples are provided to illustrate the computational model construction and the results of such an approach.

Mechanobiology of cells, vesicles and biomembranes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INTERPLAY OF ACTIVE SELF-ORGANIZATION IN DENSE NEMATIC CYTOSKELETAL STRUCTURES AND CELLULAR SHAPE CHANGES

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ABSTRACT

Endothelial cells respond to both internal and external mechanical stimuli. Forces within the cytoskeleton and cell-substrate interactions regulate their elongation. This study examines the interplay of these forces in cellular alignment using mathematical modelling. In this work, we formulated a coarse-grained active nematic model that accounts for the viscoelastic properties of the actin network, active forces from bundling proteins, actin turnover, interactions between the actin network and the extracellular matrix via focal adhesion complexes, and contrasts between isotropic and bundled nematic actin networks. We investigate low and high-friction substrate regimes. In each regime, the numerical solution of the model reveals the internal mechanism involved in the progression of cell elongation. Initially, within a circular, well-spread cell configuration, a retrograde flow of transverse and radial stress fibres emerges due to a symmetry-breaking phenomenon. These bundles are highly contractile and give rise to anisotropic contractile forces. These contractile anisotropic forces in stress fibres, along with their interaction with the substrate, lead to alignment in the overall cellular morphology. Furthermore, the mathematical model shows that cell elongation is small on soft substrates, but it is pronounced on high-stiffness substrates due to the formation of a large number of focal adhesions. This allows the stress fibres to exert higher anisotropic forces on the cells, creating more pronounced elongation. Our model effectively predicts both the cellular shape and the internal structure of the actin cytoskeleton, showing good qualitative agreement with experimental observations on endothelial cells.

Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

OPTIMIZING TEMPERATURE UNIFORMITY IN AN INDUSTRIAL SIZE ELECTRIC FURNACE: A COMPUTATIONAL FLUID DYNAMICS APPROACH

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ABSTRACT

Large size industrial furnaces are crucial in producing steel with specific mechanical properties, notably hardness. This hardness across different steel block zones is intricately linked to the temperature and duration of exposure in each zone [1]. Achieving uniform heat transfer distribution, and thus uniform temperature, is vital for desired hardness levels. Heat transfer in these furnaces takes place via radiation, absorbed by blocks' surfaces, and convection, by the internal flow pattern.
In this study, a comprehensive Computational Fluid Dynamics (CFD) simulation was conducted to study temperature evolution in an industrial size heat treatment furnace used in steel industry. The focus is on a furnace design with three ceiling-mounted axial fans, operable between 800 and 1800 rpm.

For the simulation purposes, the unsteady SIMPLEC algorithm for pressure-velocity coupling in compressible flow, the realizable k-ε turbulence model, and the DO radiation model were used. The simulation, refined through a mesh study to a 4.7 million cell mesh, demonstrated a maximum of 4.5% error in temperature readings compared to actual data from an instrumented loading cycle. This cycle involved two high-strength steel blocks, each weighing approximately 29 tons, stacked atop each other [2]. The simulation revealed that the upper block experienced a surface temperature non-uniformity reaching 236°C and a surface-to-center variance of 222°C, while the lower block exhibited a surface non-uniformity of 221°C and a surface-to-center difference of 202°C.
The study methodically analyzed the effects of fans' rotation speed and distance from the furnace ceiling, examining fans' speeds from 0 to 2500 rpm and distances from 10 to 60 cm. Results showed that 1750 rpm minimized temperature non-uniformities. Deviations from the 1750 rpm, whether higher or lower, led to more significant non-uniformities: up to 20.5°C at 0 rpm and 12°C at 2500 rpm. Adjusting fans' distance to 40 cm from the ceiling significantly enhanced uniformity, reducing the upper block's maximum non-uniformity by up to 14.5°C and the lower block's by up to 17°C. The study concludes that fans' rotation speed primarily impacts the upper block's temperature distribution, while fans' distance from the ceiling affects the lower block more significantly.

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Computational co-design of part geometry and material properties for metal additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MATERIAL-INTEGRATED DESIGN OPTIMIZATION THROUGH PROBABILISTIC PROPERTY DISCOVERY

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ABSTRACT

Existing computational design paradigms, such as shape/topology optimization, are traditionally rooted in a material-first approach, where the selection of materials precedes the actual design and optimization process. In other words, the materials are treated as predefined inputs into the design process, confining the exploration to the mechanical and physical properties that these materials inherently possess. Such a sequential process of choosing materials based on availability and familiarity, followed by designing within their constraints greatly narrows the design space. It limits innovation to the existing catalog of materials, often forcing designers to make trade-offs between material properties and the envisioned structural performance. We present a material-integrated design optimization (MIDO) approach to enable efficient discovery of novel properties tailored to a part's geometry and its operational objectives.
To push the boundaries of what is possible with existing alloys, we present a material-integrated design optimization (MIDO) approach, comprising two phases: (1) the property discovery (PD) phase, which will search for the best part designs for performance and durability, using candidate material properties deemed realizable with high likelihood, and (2) the recipe realization phase, that will find the best recipe (i.e., composition and thermal history) to fulfill the target properties, while accounting for deleterious phases and supply chain risks.
In this project, we focus on the formulating and developing the PD phase. While the PD phase need not be burdened with how exactly the properties are realized, it must be constrained by how likely it is for the material to exist. The goal is to develop the mathematical and computational foundations for concurrent optimization of material and shape by considering material properties, referred to as property bundles as explicit, independent, and continuous design variables. Our proposed approach enables rapid exploration of the expanded design space of alloy properties within reasonable feasibility bounds imposed with respect to known materials. Specifically, we (a) present a gradient-based optimization framework to enable automated discovery of properties, a.k.a. property bundles. In this view, the underlying design representation is expressed as a collection of property bundles, (b) impose a global property feasibility constraint based on a differentiable probabilistic function that controls the novelty aggressiveness/conservatism of the optimized property bundles, and (c) demonstrate the effectiveness of our approach through benchmark examples in 2D and 3D.

Multi-scale, multi-rate damage and fracture: Models, experiments, and simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PRECISION IN PREDICTION: A COMPREHENSIVE STUDY OF MASS TIMBER SFRS THROUGH FULL-SCALE COLLAPSE TESTING

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ABSTRACT

The understanding of the collapse dynamics in earthquake engineering plays a crucial role in their incorporation into building standards. This investigation originates from a groundbreaking series of mass timber building projects carried out on the world's largest outdoor shake table in San Diego, California, spanning the years 2022-2024 (NHERI Tallwood and NHERI Converging Design projects). After extensive full-scale testing, including the ten-story Tallwood and six-story Converging Design, the upper stories were deconstructed, transforming the taller structure into a representative three-story collapse test specimen. The post-tensioning of the original walls was reconfigured to ensure consistency with a potential design specification proposal. This presentation specifically explores the comparison between the results of full-scale collapse tests, focusing on the seismic force-resisting system (SFRS) of the three-story building, and the numerical predictions formulated prior to the test through nonlinear time history analysis. The SFRS incorporates mass timber panels as rocking walls and U-shaped flexural plates (UFPs) within each story level, augmenting energy dissipation capabilities. Additionally, post-tensioning rods provide re-centering for each wall, and the specifically designed integration of floors and rocking walls effectively uncouples lateral and vertical movements. Through a detailed examination of the modeling intricacies, this presentation aims to contribute valuable perspectives on accurately predicting the behavior of innovative SFRS during severe shaking to better inform margins against collapse.

Multiscale methods for advanced manufactured materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING ADDITIVELY MANUFACTURED METALLIC MICROSTRUCTURES FOR DYNAMIC RESPONSE

John Mitchell[1], Stewart Silling[1], Edwin Chiu[1], Stephen Bond[1] and Timothy Ruggles[1]*

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ABSTRACT

Additive manufacturing of metals produces material microstructures which are inherently different from those of wrought materials as they arise from a complex temperature history associated with the additive process. Because of complex microstructure morphologies and spatial heterogeneities, material properties are heterogeneous and reflect underlying microstructure. This paper describes a workflow for simulating the dynamic and spall response of additively manufactured metals [1]. The approach consists of simulating microstructures associated with the additive manufacturing process, methods for representing spatially heterogeneous microstructures on a peridynamics discretization, and a specialized material model for handling dynamic material failure under spall conditions. Material properties are spatially distributed onto the discretization so that microstructure effects arising from additive manufacturing can be systematically incorporated into engineering scale calculations. Model simulations are compared with laboratory flyer plate test data.

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Fluid-structure interaction in interface and moving boundary problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GENERALIZATION OF GHOST CELL BOUNDARY MODEL FOR PARTICLE-BASED SIMULATION OF WAVE–STRUCTURE INTERACTIONS

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ABSTRACT

This study proposes a highly accurate ghost cell boundary (GCB) model [1] for mesh-free particle methods that applies semi-implicit time integration including stabilized incompressible smoothed particle hydrodynamics (ISPH) [2]. The GCB model enables us to directly use meshes such as finite elements as the wall boundary of complex shapes and be suitable for fluid–structure interaction analysis using both mesh-free particle and mesh-based methods. However, conventional GCB model does not satisfy wall boundary conditions strictly, and is limited in its scope of application to particle methods with explicit schemes. Our proposed method is applicable to semi-implicit type particle methods including the stabilized ISPH and can use an arbitrary number of integration points. We also clarify how to apply formulation of the fixed ghost particle [3] to the integral points of the GCB model and realize the strict imposition of the wall boundary condition. We conduct wave–structure interaction problems and validate the accuracy and applicability of the proposed method by comparing numerical results with experimental ones.

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Advances in computational mechanics for flow-induced vibrations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FROM WAVE-POWERED PROPULSION TO FLIGHT WITH MEMBRANE WINGS: INSIGHTS POWERED BY HIGH-FIDELITY IMMERSED BOUNDARY METHODS BASED FSI SIMULATIONS

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[1]Johns Hopkins University

ABSTRACT

The perpetual advancement in computational capabilities, coupled with the continuous evolution of software tools and numerical algorithms, is creating novel avenues for research, exploration, and application at the nexus of computational fluid and structural mechanics. Fish leverage their remarkably flexible bodies and fins to harness energy from vortices, propelling themselves with an elegance and efficiency that captivates engineers. Bats fly with unparalleled agility and speed by using their flexible membrane wings. Wave-assisted propulsion (WAP) systems, utilizing elastically mounted hydrofoils, convert wave energy into thrust. Each of these problems involve a complex and elegant interplay between fluid dynamics and structural mechanics. Historically, investigations into such phenomena were constrained by available tools, but modern computational advancements now facilitate exploration of these multi-physics challenges with an unprecedented level of fidelity, precision, and realism. In my presentation, I will discuss projects that harness the capabilities of high-fidelity sharp-interface immersed boundary methods to address a spectrum of engineering and biological challenges involving fluid-structure interaction.

PSE (Problem Solving Environment)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADVANTAGES OF 500 HZ MONITORS IN E-SPORTS

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ABSTRACT

Computer monitors work on 60 Hz generally, but higher refresh rates of 240 Hz and 350 Hz are used for e-Sports. In 2023, 500Hz displays were launched on the market in the U.S. in 2023. We have been investigating whether using a display with a high refresh rate has an effect on winning or losing in e-sports. As a preliminary investigation, we conducted a simple reaction test, pressing a button as fast as possible when the color of the display changed. The results showed that most people were able to respond to high refresh rates regardless of their game skill[1].

In addition, the effect of monitor refresh rate on gaming in a complex shooter game was examined in two subjects. First, both players fought with a 360-Hz frequency monitor, and their respective win rates were used as their reference win rates. Second, the players played against each other with 360-Hz monitors versus monitors below 60 Hz, and the player with the 360-Hz monitor recorded a win rate that was 10 to 20% higher than the reference win rate. The present study will examine whether these results are similar when using a 500 Hz monitor.

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Novel numerical approaches for integrated disaster simulation for digital twin from living spaces to urban scales
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SEISMIC RESPONSE ANALYSIS OF A NUCLEAR POWER PLANT USING A 3D HIGH-FIDELITY FE MODEL WITH A TENSION CRACK MODEL FOR CONCRETE MATERIAL

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[4]*Science and Disaster Resilience*

ABSTRACT

In previous studies, the authors conducted finite element (FE) seismic response analyses using a high-fidelity integrated model of a nuclear power plant. The high-fidelity finite element mesh employed tetrahedral elements for components such as the pressure vessel, containment vessel, suppression chamber, vent pipes, various supports, and the reactor building. In this study, the concrete material within the reactor building and support structures, including the pedestal of the pressure vessel, is represented using a concrete constitutive model with a tensile crack model proposed by Yamashita et al. Subsequently, a seismic response analysis using the FE model is executed on the supercomputer Fugaku. The analysis reveals numerous tensile cracks in regions experiencing tensile stress.

Computational methods in environmental fluid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT OF TRAFFIC NOISE EVALUATION SYSTEM USING FINITE ELEMENT METHOD

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ABSTRACT

Noise is one of the seven major types of pollution in Japan, and it leads to the highest number of complaints according to a survey published by the Ministry of Internal Affairs and Communications in December 2023. There have been presented a number of numerical methods to evaluate the traffic noise. Based on the frame of reference used, those methods can be classified into two categories: 1) Methods based on the geometrical acoustic theory and 2) Methods based on acoustic wave theory. Both methods have advantages and disadvantages. For geometrical acoustic theory methods, the CPU time is very short but the numerical accuracy is low comparing with the methods based on the acoustic wave theory. On the other hand, the method based on the acoustic wave theory gives accurate solution but the simulation becomes a large scale simulation.

This paper presents a noise evaluation system based on acoustic theory. The finite element method is employed for unsteady wave equations, which is suitable for arbitrary shapes and has excellent applicability to non-uniform materials. The 3D wave equation is employed for the governing equation and the Perfectly Matched Layer (PML) method [1] is utilized as a treatment method for boundary condition. In order to consider multiple moving sound sources such as a traffic noise, a time-variant convolution method [2] is introduced. In addition, the transmittance and reflectance are evaluated by performing the analysis taking into account the microscopic structure within the sound barrier. The auralization method based on VR technology is also introduced to understand the noise level intuitively.

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New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN TOPOLOGY DESIGN FOR TURBULENT CHANNEL FLOW

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ABSTRACT

Topology optimization technology using the gradient method has traditionally been applied to create new concepts to improve the competitiveness of products.However, gradient-based topology optimization can fall into a local optimum, and its calculations are often unstable for complex flow fields in actual products. Therefore, it is important to construct a method that can stably search a wide range without gradient information. In this study, we focus on data-driven topology design, which can search for diverse shape designs based on the combination of a genetic algorithm and a deep generative model. This approach enables gradient-free topology optimization under a high degree of design freedom from initial shape given by parametric designs and topology-optimized designs using low-fidelity models.In this study, we apply the approach to turbulent channel flow. In addition, regarding the concept extracted from the obtained shape, we demonstrate the relationship between shape and pressure loss through the numerical example.

AN ATTEMPT TO CONSTRUCT A RESPONSE DATABASE FOR THREE-DIMENSIONAL FRAME MODELS

Yasunori Mizushima[*1], Masaki Gohara[2], Takuma Kawakami[3], Motoki Uchiyama[3], Motonobu Maekawa[3], Shuei Ikeda[3], Motoki Akazawa[3], Sota Murashima[1] and Yasuyuki Nagano[2]*

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[3]*Takenaka Corporation*

ABSTRACT

Recent advances in computing technology enable seismic response analyses of buildings using not only mass-spring models but also three-dimensional frame models. Mass-spring models are widely used in time-history response analysis in Japan because of their simplicity and low computational cost. However, we believe the mass-spring models are accurate enough to represent buildings due to the simplification, especially for geometrically complex buildings. Conversely, three-dimensional frame analysis, which models the structure of a building by replacing columns and beams with linear elements of specified cross-sectional properties connected at nodes, allows for a more detailed understanding of response behavior. The demand for such three-dimensional analysis has increased in recent years due to some reasons. For example, there is a need to understand the nonlinear behaviors of each member of buildings subjected to long periods and duration seismic ground motions.

However, three-dimensional frame models require numerous input parameters and output data. The number of variables makes it difficult to extract correlations and causal relationships. This study attempts to construct a response database for three-dimensional frame analysis including both the input variables and the results. The input variables were randomly generated. A base model was designed using integrated structural design software, and the parameters of the base model were tuned based on the input variables database. The structural analysis was conducted using LS-DYNA, which is commonly known as high-efficient parallel nonlinear structural analysis software by adopting the explicit time integration scheme. As output data, the maximum story drift, story shear force, and so on were extracted and stored in the database. On the response data, basic statistical analysis, multiple regression analysis, and clustering by the t-SNE method were performed. From the statistical analysis, the response of the building is related to the column dimensions.

This study represents a first step in enabling designers to comprehend complex and large-scale analysis models, leading to more effective and efficient building designs. Through statistical analysis, we were able to derive simple relationships between input and output, a finding we consider crucial as a foundational step. As a further step, we aim to conduct various analyses to comprehend the relationship between building characteristics and seismic responses.

Machine learning methods for multiscale and multiphysics material modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NEW PARADIGM FOR MULTIPHYSICS AND NON-LINEAR MECHANICS MODELING: INTEGRATED FINITE ELEMENT NEURAL NETWORKS (I-FENN)

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[1]*New York University Abu Dhabi*

ABSTRACT

The growing complexity of the phenomena sought to be modeled using computational mechanics tools is leading to an unprecedented need for more sophisticated coupled models. Such models are encountered by many challenges, one of which is their tremendous computational cost. The recent advances in scientific machine learning (SciML) have been more frequently investigated as possible alternatives to more established numerical methods, such as FEM. While SciML models have shown some tangible promising results in the field of computational mechanics, they suffer from fundamental shortcomings that currently prevent them from becoming rigorous and reliable alternative numerical solvers as standalone methods.

These challenges have inspired our group to establish a new method coined as Integrated Finite Element Neural Network (I-FENN). The proposed method attempts to couple traditional FEM solvers with the newly established deep learning approaches. The fundamental idea is to decompose coupled problems in a way that allows a neural network to predict one aspect of the physical processes, then integrate the network prediction within a generic FEM solver in a fashion that resembles a typical user-defined material model. The resulting coupled solver is expected to be much faster than traditional mixed FEM thanks to the smaller sized system of equations, and possibly faster convergence in the case of non-linear models. We herein present two applications of I-FENN: modeling gradient non-local damage mechanics and fully coupled transient thermoelectricity.

In the case of gradient damage, a neural network is first trained to predict the non-local strain from local strain, thus representing the solution of gradient non-local diffusion equation. The network output of non-local strain is then integrated within a local damage solver system. Thus, the resulting I-FENN algorithm provides the solution of a non-local damage model at the reduced cost of a local one. In the case of transient thermoelasticity, the network is trained to predict the temperature based on the solution of the balance of heat energy equation. The output temperature is then fed into the traditional FEM solver of the balance of momentum. Hence, the resulting I-FENN solver solves the coupled thermoelasticity model at the cost of uncoupled model. Various types of networks have been investigated including physics-informed, temporal convolution networks, and variational-based networks. The presentation will include the various types of networks developed, investigation of their convergence and numerical behavior, and efficiency and scaling of the computational savings as the investigated models grow.

Immersed-boundary variational methods: Theory, data structures, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ASSESSMENT OF UNFITTED FINITE ELEMENT METHODS FOR FLUID-STRUCTURE INTERACTION OF FLOATING OFFSHORE STRUCTURES

Jan Modderman[*1] and Oriol Colomés*[1]

[1]*Delft University of Technology*

ABSTRACT

To transition towards a carbon neutral future, we are required to look for new sources of renewable energy. The potential of the sea for capturing renewable energy is immense, but it requires us to move towards deeper waters. Therefore, there is an increased demand for research into floating renewable energy capturing devices which are accompanied by their own unique challenges. One driver in further increasing the feasibility of floating energy capturing devices is an increase of fidelity and efficiency in modeling of Fluid-Structure Interaction (FSI) problems involving free surface flows and floating bodies. One of the main issues in computational FSI for floating renewables is the need to deal with complex structural geometries. This is especially relevant in the design optimization phase, where an optimal structural solution must be defined for site-specific conditions in a limited time. Unfitted/immersed/embedded Finite Element (FE) methods are convenient for these situations, avoiding the need of ad-hoc mesh generation.The challenge here is how to deal with an unfitted structure that interacts with free surface flows.

In this talk we will present a single-phase FE approach for free surface flows, where only the wave-structure interaction is accounted for, in combination with an unfitted floating structure with arbitrary geometry. In this work we propose a monolithic method, ensuring robustness and efficiency of the solution, for several unfitted FE methods. We will demonstrate the capabilities of the proposed framework with a series of tests for wave-structure interaction problems for offshore engineering applications, assessing accuracy and conservation properties. Lastly, we will compare the performance of the following unfitted FE methods, namely CutFEM [1], AgFEM [2] and (W)SBM [3].

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[3] Oriol Colomés, Alex Main, Léo Nouveau, and Guglielmo Scovazzi. ”A weighted Shifted Boundary Method for free surface flow problems.” Journal of Computational Physics 424 (2021): 109837.

SYMBOLIC REGRESSION VIA NEURAL NETWORKS

Jeff Moehlis[*1], Nibodh Boddupalli[1] and Tim Matchen[1]*

[1]*University of California, Santa Barbara*

ABSTRACT

Identifying governing equations for a dynamical system is a topic of critical interest across an array of disciplines, from mathematics to engineering to biology. Machine learning—specifically deep learning—techniques have shown their capabilities in approximating dynamics from data, but a shortcoming of traditional deep learning is that there is little insight into the underlying mapping beyond its numerical output for a given input. This limits their utility in analysis beyond simple prediction. Simultaneously, a number of strategies exist which identify models based on a fixed dictionary of basis functions, but most either require some intuition or insight about the system, or are susceptible to overfitting or a lack of parsimony. Here, we present a novel approach that combines the flexibility and accuracy of deep learning approaches with the utility of symbolic solutions: a deep neural network that generates a symbolic expression for the governing equations. We first describe the architecture for our model and then show the accuracy of our algorithm across a range of classical dynamical systems.

This is joint work with Nibodh Boddupalli and Tim Matchen, and has appeared in Chaos, 33: 083150 (2023).

PROJECTOR ASSEMBLY: BRIDGING POISSON AND ELASTICITY FORMULATIONS

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ABSTRACT

Virtual element methods define their shape functions implicitly (tailored to each element's geometry), foregoing the typical reference element and transformation scheme usually employed by the finite element method. The formulation leverages the use of polynomial projections supplied by heuristic stabilizations when necessary. These projections are represented by projector matrices, which require the solution of a local system. Elasticity formulations usually employ an L2-projection from a displacement multifield onto a strain multifield, requiring the solution of a considerably larger system than a typical Poisson problem would require, with dense matrices and lots of zeroes. This work presents a way to obtain the projections for elasticity formulation by assembling from the L2-projection for each derivative of the one-field a Poisson formulation, resulting in smaller local systems being solved and more efficient storage. This approach is based on the linearity of both projections and derivatives, and is shown in the examples to preserve the convergence rate of the method.

Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFICIENT AND ACCURATE THERMOMECHANICAL MODELING OF FUSED FILAMENT FABRICATION PROCESS

Satyajit Mojumder[*1] and Wing Kam Liu*[1]

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ABSTRACT

Process modeling plays a significant role in process optimization and in-situ process control for defect mitigation and part qualification. Here, we present a GPU-accelerated and higher-order accurate thermomechanical modeling of the fused filament fabrication (FFF) process for thermal response and residual stress of the printed part. The higher-order accuracy compared to finite elements is achieved by implementing a new deep learning-based computational theory called Convolution-Hierarchical Deep-learning Neural Network (C-HiDeNN) [1] where a customized neural network architecture is used for incorporating nonlinearity in the calculation. C-HiDeNN is computationally efficient as it requires less degrees of freedom for similar accuracy of FEM and a higher convergence rate. Also, the high-temperature gradient during the FFF process can be captured more accurately using C-HiDeNN approach. The C-HiDeNN FFF process is validated against the experimental results and investigated for various process parameters such as nozzle speed, nozzle temperature, layer thickness, raster distance, bed temperature, and tool path orientation in this study. The FFF process modeling tool not only provides guidance for choosing appropriate process parameters but also optimizes it for desired part performance. In addition to accuracy, C-HiDeNN allows the creation of a differential simulation capability for FFF process optimization. These data-driven modeling and simulation capabilities provide new opportunities for developing novel material systems and their process optimization using the FFF process.

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Fluid-structure interaction: Methods and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A FINITE-ELEMENT BASED METHOD FOR THE INTERACTION OF FLUIDS WITH EVOLVING BEDFORMS

Jorge Molina[*1] and Pablo Ortiz*[1]

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ABSTRACT

Prediction of fluid-terrain interactions involving the transport of cohesionless sediment is fundamental for understanding the morphodynamics of natural systems and its effects on civil structures. However, the simulation of such phenomena is challenging due to the necessity of handling several interfaces, including fluid/erodible layers, erodible/non-erodible layers, fluid/non-erodible layers and, in the case of multiphase flows, interactions between different fluids [1].
This work introduces a continuous finite element model to reproduce the fluid flow-bedform interaction. The approach employs a Non-oscillatory Finite Element Method (NFEM) to solve both the complete Navier-Stokes equations [2] and the fluid-bedform interface evolution. This evolution occurs due to spatially non-balanced sediment fluxes and is addressed through the solution of a conservation equation for the erodible layer thickness. Sign preservation is particularly relevant for landform tracking when interfaces limiting with non-erodible beds are present, thus ensuring the positivity of the erodible sediment layer thickness [3]. Besides, the fluid/terrain interface is explicitly captured through a surface tracking methodology. First, new nodes fitting the interface are incorporated into the finite element mesh, then elements beneath this interface are deactivated while intersected elements are restructured to get a mesh composed exclusively of tetrahedral or triangular elements.

Numerical experiments demonstrate capabilities of the method by exploring relevant problems related with civil engineering, such as the evolution of dunes and trenches, the scour of submerged piles and dam-break type problems on erodible beds.

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Current trends in phase-field modeling and computations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CHEMO-HYDRO-MECHANICAL VARIATIONAL PHASE-FIELD FRACTURE MODEL

Mostafa Mollaali[*1], Renchao Lu[1], Vanessa Montoya[2], Keita Yoshioka[3] and Olaf Kolditz[1]*

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ABSTRACT

We present a chemo-hydro-mechanical variational phase field model for simulating fracture initiation and propagation. By employing a staggered approach, we couple three key subprocesses: (i) fluid flow in porous media, (ii) reactive transport, and (iii) mechanical deformation/fracturing of porous media. In our approach, we integrate the geochemical package PHREEQC [1] within an operator-splitting framework, coupled with a finite element transport solver to compute chemical reactions in thermodynamic equilibrium (dissolution or precipitation) that alter the porosity.

To account for the mechanical damage caused by the chemical reaction, a variable is introduced into the constitutive relation, representing the degree of chemical damage ranging from 0 (indicating intact material) to 1 (indicating damaged material) [2]. Furthermore, we consider the influence of fractures and changes in porosity on both hydraulic conductivity [3] and the effective diffusion coefficient [2].

We verified our model through benchmark examples in capturing fracture initiation and propagation resulting from chemical reactions. The implementation of the proposed model was carried out within the open-source finite element framework OpenGeoSys. The research work is part of the EURAD project.

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Multiscale computational and data-driven approach of advanced materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE MODELING OF SHORT HYPERELASTIC COMPOSITE RODS: APPLICATION TO ELASTOMERIC ISOLATORS

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ABSTRACT

Elastomeric isolators have been used extensively for the seismic protection of new and existing structures. Extensive research has been done regarding the hysteretic behavior of these devices, and several phenomenological models have been proposed to predict their behavior. The nonlinear geometric effects have also been extensively studied from an experimental perspective, but their numerical implementations have been restricted to simplified models. Today, even the most widely used numerical models for rubber isolators are discrete spring models in which the isolator is treated as a rigid element connected by discrete springs representing their axial, rotational and shear stiffness. The definitions of these springs are manipulated analytically such that the model captures fundamental behaviors such as the buckling of the isolators. This approach presents drawbacks for capturing some behaviors of the isolators, such as accurately predicting the local stresses which are important in predicting the cavitation under tensile stress (or detachment in the case of unbonded elastomeric isolators), as well as incorporating the response for non-standard boundary conditions such as supports under rotations. In this study, a fully mechanical multiscale model for elastomeric isolators is proposed that considers the continuous deformations in the isolator while also accounting for the periodic microstructure formed by the alternating rubber and reinforcement layers. At the macroscale, the isolator is treated as a one-dimensional continuous Cosserat rod which allows for finite deformations. At the microscale, a unit cell formed by a single rubber layer and two half-thickness reinforcement layers is analyzed using finite element simulations; different alternatives with varying levels of complexity, computational cost and accuracy are evaluated for the analysis of the microscale response. The proposed model is compared against high-fidelity finite element simulations and results from previous experimental programs, showing promising results.

Advancing computational mechanics with symbolic regression
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CHARACTERIZING THE COMPLEX DEFORMATION OF TIN USING GENETIC PROGRAMMING TO PERFORM SYMBOLIC REGRESSION

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ABSTRACT

Plastic deformation of β-tin (Sn) is significantly affected by strain-rate and temperature. Consequently, different experimental procedures are needed to characterize the deformation behavior of this material, especially since the changes in behavior are observed over a large range of temperatures and strain-rate regimes that span multiple orders of magnitude. This complex behavior exhibited by tin poses significant challenges when attempting to fit the observed behavior to traditional, fixed-form, empirical models. This often limits the model's applicability to specific temperature and strain-rate regimes. In this work, we address this impasse by leveraging genetic programming in order to perform symbolic regression to establish a set of data-driven models that are valid across multiple strain-rate and temperature regimes. These models are trained on a set of compression tests and split-Hopkinson pressure bar (SHPB) tests at various strain rates and temperatures. We leverage the analytical nature of the resultant models to integrate them into a continuum dynamics simulation code and perform Taylor impact simulations to demonstrate the validity of the developed models. Finally, a comparison of the data driven model predictions against conventional strength models is presented.

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Numerical modeling of granular and multiphase flows
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VALIDATING FLUID-PARTICLE INTERACTION MODELS IN DENSE GRANULAR FLOWS: A PEPT-MEDIATED APPROACH

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ABSTRACT

Dense granular flows are prevalent in industries (such as mining and pharmaceuticals) and natural disasters (including landslides and tidal waves). Enhancing the understanding of these flows is crucial, both financially and environmentally. Unfortunately, the absence of a constitutive law governing their rheology necessitates using dimensional analysis for insight. Rheological models proposed by researchers like Jop et al (2005) and Pahtz et al (2019) incorporate dimensionless numbers as functions of dynamic properties like pressure and granular temperature. These dynamic properties, occurring at the momentum transfer timescale (10-6s), are challenging to measure experimentally, leading to reliance on numerical methods like the Discrete Element Method (DEM) for understanding.

DEM, traditionally tracking individual particle movements, can be extended using techniques like Smoothed Particle Hydrodynamics (SPH) or liquid bridge modelling to account for fluid effects. SPH simulates fluid as particles, whereas liquid bridge modelling considers capillary forces between particles. Both approaches hold promise in dense granular systems, offering unique advantages. SPH captures fluid behaviour more explicitly, while liquid bridge modelling provides a detailed representation of inter-particle forces, enhancing the overall understanding of fluid-particle interactions in these complex systems.

Despite the advancements in numerical techniques, there remains a notable gap in the literature concerning experimental validation which limits our confidence in the predictive capabilities of these models. Positron Emission Particle Tracking (PEPT) is a nuclear imaging technique capable of tracking particles with millisecond temporal and millimetre spatial resolution. Coarsening these outputs, using carefully selected representative voxel elements, allows for a continuum description of kinematic fields.

This study employs PEPT to validate—or select—a suitable method (either SPH coupled or considering liquid bridge forces) for describing fluid effects on DEM. Rotating drum experiments, featuring a 460mm diameter and 200mm length, are conducted using a 50% volume filling of 10mm glass beads (DEM particles) in a water-glycerol suspension with a viscosity of 0.011 Pas. Rotational speeds, covering a range of Froude regimes, provide insights into the behaviour of dense granular flows subjected to fluid forces and the appropriate modelling thereof.

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Pähtz, T., Durán, O., De Klerk, D.N., Govender, I. and Trulsson, M., 2019. Local rheology relation with variable yield stress ratio across dry, wet, dense, and dilute granular flows. Physical review letters, 123(4), p.048001.

Imaging-based methods in computational medicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THB-SPLINE BASED VOLUMETRIC FITTING USING DIFFERENTIABLE PROGRAMMING

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ABSTRACT

Converting imaging data from different modalities into computational models that are suitable for analysis is a major challenge in the biomedical field. Geometric primitives like tetrahedra and hexahedra are commonly used to create volumetric meshes for both geometric and analytical applications. Isogeometric Analysis has revolutionized the field by providing an alternative to conventional finite element methods. By utilizing high-order spline models to describe geometry, a more straightforward and precise method is achieved. Although previous studies, such as NURBSDiff [1], have made progress in this field, they do not specifically tackle the difficulties associated with volumetric spline fitting. Conventional tensor-product splines, such as B-splines and NURBS, are not efficient in improving geometric accuracy because they do not have the ability to locally refine, resulting in a compromise between accuracy and efficiency. The objective of this study is to create a computationally efficient and precise framework for fitting volumetric CAD models that are suitable for Isogeometric Analysis (IGA) to unstructured point clouds. Truncated Hierarchical B-splines (THB-splines) utilize local refinement in tensor-product B-splines. Building upon our existing surface fitting framework [2], we have expanded the application of differentiable programming to volumetric splines, emphasizing the following key contributions. We have developed a novel differentiable THB-spline module that can be easily integrated into existing computational frameworks. This module is designed specifically for volumetric fitting. We have also conducted a thorough investigation of local refinement strategies, with a focus on optimizing them for volumetric fitting. Additionally, we have extensively tested and validated our module by applying it to 3D imaging data from biological models. Through this testing, we have demonstrated the effectiveness of our module on raw point cloud data. This work not only improves the accuracy in modeling biomedical imaging data but also makes a significant contribution to the broader field of Isogeometric Analysis by providing a more sophisticated and efficient method for volumetric CAD modeling.

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Battery modeling and computation: From material to device
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ENHANCING IONIC CONDUCTIVITY IN ASSBS THROUGH OPTIMIZED SOLID ELECTROLYTE DISTRIBUTION: A COMPUTATIONAL ANALYSIS OF THE DRY MECHANICAL MIXING PROCESS

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ABSTRACT

This study utilizes advanced computational modeling to refine the mechanical mixing (MM) technique for producing cathode composites in all-solid-state batteries (ASSBs). The main focus is on achieving uniform integration of solid electrolytes (SE), which is crucial for efficient ionic and electronic conductivity. By using finite element analysis, we quantitatively evaluate how MM optimizes SE distribution, outperforming traditional methods. Our computational approach not only predicts the formation of efficient ionic pathways but also assesses the structural integrity of cathodes under operational stresses. The findings suggest that the MM process is a scalable and computationally informed strategy for enhancing ASSB performance through meticulous cathode design and SE homogeneity.

Multi-scale, multi-rate damage and fracture: Models, experiments, and simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A COMBINED CRYSTAL PLASTICITY, HIGH ENERGY DIFFRACTION MICROSCOPY, AND MICRO-TOMOGRAPHY STUDY OF FATIGUE IN A NICKEL TITANIUM ALLOY

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ABSTRACT

Fatigue indicator parameters are a computational tool for materials design that determine the driving force for fatigue fracture and are useful in ranking deleterious microstructural features when designing engineering alloys. Many of these parameters were formulated over three decades ago (mostly for steels) using analytical models and 2D microscopy. This study revisits this development for a nickel titanium alloy using modern computational and experimental tools including computational crystal plasticity, 3D high energy diffraction microscopy (HEDM), and 3D micro-tomography. The stress state that drives fatigue fracture is shown via HEDM and mapped to fracture locations measured via micro-tomography. Computational crystal plasticity is used to elucidate the nonlinear and nonlocal mechanisms driving fatigue fracture and formulate a fatigue indicator parameter that describes fatigue fracture in a nickel titanium alloy.

Multiscale methods for advanced manufactured materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MULTISCALE MODEL FOR DISORDERED BIOPOLYMER GELS

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ABSTRACT

Due to their unique properties, biopolymer gels find extensive use in the food industry and various biomedical applications including tissue engineering. Contrary to rubber-like materials, the constituent chains in biopolymer gels aggregate through physical, rather than covalent, cross-linking. Disordered biopolymer gels exhibit two principal regions: the disordered zone containing coiled chains, and the ordered zone manifesting in the form of ion-mediated aggregation of chain segments. The resulting network combines these two regions, where the ordered structures serve as rigid junction zones between the flexible disordered chains. While there is a wealth of macroscopic studies on disordered biopolymer gels using phenomenological models, here we present a multiscale model that bridges statistical mechanics analysis on the micro-scale and prediction of mechanical properties on the macro-scale.

The constitutive relation of disordered biopolymer gels is established by integrating the micromechanics of coil-rod structures with the well-known eight-chain network model. The coil and rod respectively represent the disordered and ordered zones, and the length of each zone can change as a result of zipping (increased ion-mediated aggregation) and unzipping (reduced ion-mediated aggregation) of the junctions. Incorporating this microscopic mechanism allows the model to reproduce a phenomenon observed in previous experiments, i.e., biopolymer gels subjected to cyclic mechanical loadings exhibit hysteresis where a residual deformation remains after complete unloading. Verification of the model is performed using experimental data for alginate gels, showcasing the model's accuracy. This multiscale formulation not only contributes to an in-depth understanding of the mechanics of disordered biopolymer gels but also establishes a foundation for modelling more advanced polymer gels in future studies.

Multiphase flow and non-Newtonian fluid - Modelling and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL SIMULATIONS OF CHIRAL LIQUID CRYSTALS IN A LID-DRIVEN CAVITY USING THE LANDAU-DE GENNES THEORY

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ABSTRACT

Cholesteric liquid crystals (CLCs), also known as chiral nematic LCs, exhibit a unique helical structure with a twisted axis perpendicular to the local molecular director, characterized by the helical pitch and twist sense. This study is motivated by disruptions in the local symmetry of the director field, leading to defects in CLCs, such as deviations from the ideal helical pitch, point defects, and disclinations. These defects have significant implications for the optical and mechanical properties of CLCs, affecting light transmission, reflection, and color appearance. Understanding these effects is crucial for applications in display technologies and other fields requiring precise control of optical properties.

The objective of this study is to model, simulate, and evaluate a 2D lid-driven cavity flow of chiral LCs, investigating the effects of chiral strength (Θ), Reynolds (Re) number, and viscous flow effect (Er) on the microstructure. Employing COMSOL Multiphysics, a finite element-based commercial software package, we simulate the flow characteristics of CLCs in a 2D lid-driven cavity, utilizing the Landau-de Gennes theory for various parametric studies to explore the interconnection between the micro- and macro-structure of CLCs.

Our findings show that an increase in Re at a constant high chiral strength and low Er corresponds to heightened inertial forces, affecting the chiral structure, and subsequently increasing defects and altering overall flow patterns. Elevated chiral strength results in a chiral texture with more pronounced striations and shorter pitch lengths, contributing to an augmented presence of defects. Maintaining constant chiral strength while increasing Er disrupts the chiral structure, potentially causing fracture at very high Er. The transition from low to moderate Er increases the number of defects, while a further rise in viscous flow contribution reduces defects due to destructive effects on the chiral structure. Even under exceedingly high Er, the chiral structure and its accompanying defects persist, which is attributed to the continuous existence of a vortex where the velocity at the center is relatively small; as a result, the chiral structure and defect persist in this low–velocity region. Observations at elevated chiral strength levels reveal the emergence of a hexagonal structure adorned with penta-hepta defects, aligning with expectations based on simulations depicting the coupling between flow dynamics and structural characteristics.

Computational methods in environmental fluid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A LAGRANGIAN POSITION-BASED SPACE-TIME FORMULATION FOR FINITE STRAIN FREE-SURFACE FLOWS

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ABSTRACT

Newtonian fluids have no resistance to deviatoric stresses and can deform indefinitely. That is why most researchers adopt the Eulerian description, having as main variables the velocities in the current configuration, with indeformable spatial domain. However, Eulerian description cannot be directly applied to moving boundary flows, such as free-surface flows, multiple fluid flows and fluid-structure interaction. For some free-surface flows, a Lagrangian description can be more suitable, specially if the fluid volume is enclosed and presents only finite deformations and it makes sense to consider current nodal positions as main variables. In this work, we present a position-based space-time finite element formulation for incompressible Newtonian fluid flows using total a Lagrangian description applied to free-surface flows with finite strains. Such approach uses mixed position-pressure finite elements, with Petrov-Galerking pressure stabilization. The discretization is structured in time direction, so that the space-time shape functions are given as a tensor product of the linear space shape-functions set with the quadratic shape functions set in time direction. Thus, the space-time domain is composed of space-time slabs, that can be solved progressively, with velocities and positions in the previous slab being imposed as initial conditions on the current space-time slab. The resulting formulation is tested by numerical examples, revealing to be robust and efficient for simulating free-surface incompressible flows, like sloshing and wave propagation.

ELECTRO- AND MAGNETO-MECHANICAL COUPLING MODULATES FRACTURE IN SOFT MULTIFUNCTIONAL MATERIALS

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ABSTRACT

Smart materials are ushering in significant changes in the way humans interact with engineering devices. Numerous state-of-the-art applications are grounded in innovative methods to actuate structures that respond to various stimuli. Among these, soft dielectric electro-active elastomers (DEAP) and magneto-rheological elastomers (MREs) respond to electric and magnetic stimuli, respectively, by undergoing substantial deformations and changes in their material properties. Applications involving large deformations may lead to crack onset and propagation. In this context, the response of DEAPs to an applied electric field and the response of MREs to an internal magnetic field induced by hard-magnetic fillers with remanent magnetization can enhance the fracture behavior of such materials. Drawing on a combination of experiments and theory, we investigate the fracture behavior of an ultra-soft dielectric elastomer (~1 kPa stiffness) [1]. The application of compliant electrodes on the sides of the elastomeric samples enables the application of a high voltage during tensile deformation. Additionally, we implement a Finite Element phase-field model that addresses the multiphysics and damage evolution. The computational testbed provides a better understanding of the physical interplays driving crack onset and propagation. The results reveal that lateral Coulomb forces generate an intricate stress triaxiality state that induces beneficial crack tip blunting and reduces stress concentration. Consequently, the work to fracture increases and crack propagation is delayed. Together with the pure elastomer samples, we manufacture composite samples with BaTiO3 particles to amplify the electro-mechanical coupling. Subsequently, we examine the fracture behavior of ultra-soft MREs with remanent magnetization [2]. To achieve this, non-magnetized and pre-magnetized hMRE samples are manufactured with hard-magnetic fillers and the same ultra-soft elastomeric matrix. Here, we report crack closure due to the remanent magnetic field as a phenomenon that delays the opening of cracks. Furthermore, we introduce for the first time a bespoke multiphysics phase-field framework for fracture of hMREs. The results suggest that remanent magnetic fields induce beneficial compressive stresses in the medium, decreasing stress concentration at the crack tip.

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TWO-SCALE MODELING AND INELASTIC ANALYSIS OF CFRP FAN BLADE DOVETAILS

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ABSTRACT

Carbon fiber-reinforced plastics (CFRP) are widely being used as structural materials for aircraft because of their high specific strength, high specific stiffness, and high corrosion resistance. Recently, some jet engine manufactures have tried to use CFRP for fan blades of jet engines to improve the engine efficiency. Since fan blades are generally subjected to cyclic loads due to centrifugal force and aerodynamic force, it is important to investigate damage behavior of CFRP fan blades due to fatigue.

When investigating such behavior of CFRP fan blades, one has to pay special attention to “dovetails”. Dovetails are tapered parts at the bottom end of fan blades, and are attached to grooves on rotating shafts called “dovetail slots”. Thus, they are subjected to the above-mentioned loads most severely. It is revealed that CFRP dovetails can fracture by delamination [1].

Our research group has conducted elastic-viscoplastic two-scale analyses of CFRP laminates based on a mathematical homogenization theory, and revealed that the viscoplastic deformation in resin sections affects the fatigue behavior of CFRP laminates such as delamination [2].

In this study, inelastic two-scale analysis of a CFRP dovetail is conducted as a preparation of applying the fatigue life evaluation method to CFRP dovetails. To this end, a two-scale modeling method for CFRP dovetails is developed, and macroscopic and microscopic finite element models are created. In addition, the two-scale analysis method is implemented in the finite element analysis software Abaqus with its user subroutine function. The present method is then applied to the inelastic two-scale tensile analysis of a CFRP dovetail. The analysis results show that viscoplasitc deformation microscopically accumulates in the resin sections around the upper end of the contact surface between the dovetail and dovetail slot, which is in good agreement with the areas where delamination actually occurred in experiments [1].

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Computational methods for wind energy
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FINITE ELEMENT-BASED SIMULATION OF LARGE WIND TURBINES WAKE USING THE ACTUATOR LINE METHOD

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ABSTRACT

The numerical simulation of wind turbines and wind farms aerodynamics represents an open challenge in computational mechanics. It involves multi-physics and multi-scale phenomena, turbulent flows at very large Reynolds numbers, atmospheric boundary layer features, and rotor machinery flow features and dynamics.
The geometrically resolved Computational Fluid Dynamics (CFD) [1] is renowned to be the highest-fidelity approach for wind turbine simulations but it has still a too high computational cost if employed for wind farm flow analysis. For this application, several reduced-order models have been formulated to obtain reliable results at a sustainable computational effort. Among the others, large eddy simulation (LES) with Actuator Line Model (ALM) [2] represents a valid middle-fidelity alternative for accurately simulating the wind turbine wakes dynamics and its interaction with the atmospheric boundary layer turbulence.
Most implementations of the ALM are derived for volume-based CFD solvers. In this presentation we report the implementation of this model in a Finite Element Method (FEM) framework, which allows the use of a Variational Multiscale (VMS) model [3] instead of the standard LES formulation used in finite volumes. The ALM-VMS formulation is applied to study a 15MW wind turbine rotor, comparing the results with geometrically resolved RANS solution of the same rotor.
The presentation will show performance and results of the method in terms of aerodynamic variables of main interest, such as velocity induction fields, rotor loads and aerodynamics, near and far wake features. Through this analysis we show the main strengths and weaknesses of this implementation and its reliability with respect to a model of higher fidelity.

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Recent advances in meshfree and particle methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SMOOTHED PARTICLE HYDRODYNAMICS SIMULATION OF LANDSLIDES WITH DISCONTINUITIES

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ABSTRACT

Discontinuities are a major factor involving the initiation of soil disasters such as landslides. However, the simulation of discontinuities with the Smoothed Particle Hydrodynamics (SPH) method remains a great challenge, since this method is based on a continuum mechanics framework. This means that all numerical approximations are based on the assumption that all neighboring particles belong to the same continuum body, which is not the case when a discontinuity is initiated. In this context, we propose some modifications on the total Lagrangian SPH (TLSPH) in order to simulate the detachment of soil at the initiation of a landslide event.

The Smoothed Particle Hydrodynamics (SPH) is a numerical scheme in which the domain is discretized into Lagrangian particles, and the forces applied to those particles are calculated as a summation of the contributions of the neighboring particles. It has been widely used for fluid dynamics problems, but recently it has also been used to simulate landslides with reasonable success. In this work, we utilize the total Lagrangian version of the SPH method, which refers to the usage of the reference configuration to calculate the spatial derivatives. As a result, some problems such as the tensile instability can be fully overcome, and, consequently, it enables a much higher accuracy. However, using the reference configuration means that neighboring particles do not change, which is unfavorable for the simulations of discontinuities.

In this context, we propose a framework where particles at a discontinuity interface are detached from the main soil continuum, so they start to act as a separate soil body. In order to accomplish that, we applied Discrete Element Method (DEM)-inspired forces to enable self-contact between the detached soil bodies. The soil itself is simulated as a finite strain elastoplastic material using the Hencky hyperelastic model and the Mohr-Coulomb yield criteria. Then, we apply a limit on the plastic deformation to enable the fracture initiation. In this way, we developed a method where clear discontinuities can be simulated in a natural way.

Machine learning for design tasks and inverse problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GENERATIVE IMAGE MODEL FOR STRUCTURAL DESIGN CONSIDERING BOTH MECHANICAL PERFORMANCE AND STYLISHNESS

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ABSTRACT

In mechanical design, shapes that combine mechanical performance and design are required. For example, in the development of a vehicle, the shape of the vehicle must combine aerodynamic performance and stylishness. However, after the designer sketches the shape design, if the shape does not meet the required mechanical performance, there is a possibility that the study will be reworked. In this study, we propose a generative image model for structural design that takes mechanical performance and stylishness. The proposed model can generate images of candidate design shapes that satisfy the mechanical performance, and is expected to streamline the designer study conducted in the early planning stages of machine design. The proposed generative image model consists of two elements. The first element is the part that generates silhouettes that satisfy the mechanical performance. In this part, the silhouette of the shape is generated by considering the relationship between design variables and cost functions used in the evaluation of mechanical performance. The silhouette uses an implicit shape representation using the Signed Distance Function, and the encoder-decoder model is used to learn the input-output relationship. The second element generates a realistic vehicle design based on the obtained silhouette. In order to generate a realistic vehicle design using the obtained silhouette as a constraint, the diffusion model with ControlNet is used. This method enables the designer to check whether the design meets the mechanical performance requirements at sketch stage, which is expected to reduce the rework of the study. The validity of this method is demonstrated using numerical examples.

SUBDOMAIN EIGENMODE-DEFLATION PRECONDITIONING FOR PARALLEL FINITE ELEMENT ANALYSIS

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ABSTRACT

Deflation preconditioning in iterative methods is a technique that projects the linear system onto a space orthogonal to the deflation space by multiple linearly independent vectors, which are known in advance. The deflated conjugate gradient method, as proposed by Saad et al. [1], is an approach that applies deflation preconditioning to the conjugate gradient method.

In deflation preconditioning, there are numerous options for selecting the bases. The one of options is the eigenmode deflation, which is the method using the lower eigenmodes of the coefficient matrix. This method reduces the condition number of the problem by deflating the lower eigenmode components, which are a factor to the deterioration of convergence in iterative methods. However, unless the eigenmodes are already known beforehand, it is necessary to perform eigenvalue analysis before starting the iterations to acquire the lower eigenmodes required. The methods, such as Lanczos method and LOBPCG, are available for eigenvalue analysis, however the computational cost of calculating lower eigenmodes is generally significant. Bergamaschi has reviewed the behavior of iteration counts when using eigenmode deflation[2], but the paper has not considered the total computation time, including the acquisition of eigenmodes. The discussion remains focused solely on convergence.

Besides, subdomain deflation, a method that involves dividing the analysis domain into several subdomains and independently obtaining deflation bases in each of these subdomains, has been proposed. The bases obtained through subdomain deflation are expected to enhance preconditioning performance, as the dimension of the deflation subspace is larger compared to the bases obtained on the whole domain.

This study proposes subdomain eigenmode-deflation preconditioning, which applies subdomain deflation to eigenmode deflation preconditioning. The proposed method aims to reduce the computational cost of acquiring eigenmodes. The proposed method is applied to a parallel finite element analysis based on domain decomposition, utilizing the subdomains obtained from domain decomposition method as the basis acquisition areas for subdomain deflation. As a numerical example of a thin-plate shape model, the preconditioning performance and parallel performance are discussed.

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New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A FRAMEWORK FOR LEVEL-SET BASED TOPOLOGY OPTIMIZATION WITH CONSTRAINED SHAPE UPDATES

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ABSTRACT

We propose a framework for level-set based topology optimization which allows for highly constrained shape updates along a user-specified component of the shape boundary, together with conventional free-form shape updates along the remainder of the shape boundary. The possible constraints include requiring that the constrained component of the shape boundary must move in an affine manner, or must remain attached to a primitive geometric shape (e.g. plane, cylinder). This framework allows us to optimize the position, orientation or scaling of surface patches in the context of topology optimization. It provides a new aspect of control that is highly useful for engineering design problems, especially for multi-functional parts where certain components of the shape boundary may only be altered parametrically. For instance, the part to be optimized is required to include a circular aperture to accommodate a bolt hole or a pin joint. Our framework allows us to simultaneously optimize the aperture radius as well as the free-form shape and topology of the remainder of the part. Our work is related to previous work that seeks to find optimal locations for structural loads and supports [1] in topology optimization but operates in the level-set context, and allows for the imposition of more general affine constraints.

To generate shape updates we transport the level-set function of the shape with respect to a velocity field defined on the entire design domain at each iteration. We construct this velocity field using a novel constrained Hilbert space extension (C-HSE) method that expands upon existing Hilbert space extension methods [2] by incorporating the affine motion constraints into the variational problem. As a result, the C-HSE method generates a velocity field that is a descent direction for a user-specified objective function while ensuring constraint satisfaction. The C-HSE method allows multiple distinct regions to have different constraints, with many possible constraint types, e.g. combinations of translations, rotations and scalings. We show results on a variety of canonical problems with geometrically constrained boundaries.

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Fluid dynamics and SciML: Navigating challenges and seizing opportunities
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DATA-DRIVEN REDUCED ORDER MODELS FOR PARTITIONED FLUID-STRUCTURE INTERACTIONS

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ABSTRACT

The main goal of this work is to develop a data-driven Reduced Order Model (ROM) from high-fidelity simulation result data of a Full Order Model (FOM), in order to predict at lower computational cost, the time evolution of solutions of Fluid-Structure Interaction (FSI) problems. For some FSI applications, the elastic solid FOM (with neglected inertia) can take far more computational time than the fluid one. In this context, for the sake of performance, one could only derive a data-driven ROM for the structure and try to achieve a partitioned FOM fluid solver coupled with a solid ROM.
In this paper, we evaluate the partitioned ROM-FOM coupling on study cases with strong coupling: an incompressible 2D wake flow over a cylinder facing an elastic solid with two beams, and 3D model of the problem with a clamped solid and a nearly incompressible hyperelastic material. The accuracy and performance of the proposed ROM-FOM strategy on these cases are explored while investigating the effects of the model's hyperparameters, especially with the presence of complex/chaotic dynamics [1]. The ability to predict, not only the displacement field, but also the volumetric strain field, in the context of mixed finite elements for incompressible materials is demonstrated. In addition, we show the effect of the structural ROM on decreasing the coupling rate of convergence. To mitigate this issue, we present an additional data-driven approach, that further accelerates convergence, while implemented non-intrusively within the framework of partitioned FSI coupling and Quasi-Newton acceleration techniques [2].
We demonstrate on the considered test cases a high prediction accuracy and significant speedup achievements using our proposed strategy.
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Coupled computational mechanics: Solutions for FSI simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMPROVING PERFORMANCE OF VOLUME OVERLAP CALCULATIONS FOR COUPLED MULTI-PHYSICS SIMULATIONS

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ABSTRACT

Many physics coupling algorithms, such as the modified Immersed Finite Element Method (mIFEM) [1], involve volume intersection calculations to weight interactions of physical quantities in the overlapped solution domains. These calculations are often expensive, involving a search for overlapping discretized cells, partial volume computations, and reductions of those partial volumes for all overlapped cells. When one or more of the computational domains employs an unstructured discretization, these operations become even more costly and can dominate the runtime of a coupled simulation. Performance improvements to these algorithms can significantly impact simulation runtime and scalability.

We present recent work to improve runtime performance of the overlap computations used in the Eulerian/Lagrangian coupling of the SABLE hydrodynamics code to SIERRA/SM explicit solid mechanics code using the mIFEM approach. We compare isolated performance of the volume overlap computations before and after the improvements, and demonstrate portability of the improved algorithms to GPU architectures that are increasingly available on commodity HPC platforms. Finally, we demonstrate the impact to overall runtime of an example coupled simulation using SABLE and SIERRA/SM.

This work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories, a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525.

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Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREDICTION OF PROCESS OUTCOMES WITH UNCERTAINTY IN LASER POWDER BED FUSION ADDITIVE MANUFACTURING

Daniel Moser[*1], Nicole Aragon[1], Michael Heiden[1], Aashique Rezwan[1], Theron Rodgers[1], David Saiz[1] and Michael Stender[1]*

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ABSTRACT

Part qualification remains a key challenge to adoption of laser powder bed fusion (LPBF) technologies, particularly for high consequence applications. This work details efforts to reduce the testing burden of LPBF qualification by using physical modeling and uncertainty quantification to make process outcome predictions that account for inherent process variabilities. Beginning with detailed melt pool-scale models, LPBF machine uncertainties are estimated and propagated through a series of models to predict thermal response, melt pool morphology, porosity formation, microstructure growth, and mechanical deformation. The resulting probabilistic predictions are compared against experimental data obtained from metallography, micro-CT, EBSD, and structured light scanning measurements. Agreement with the data is assessed and gaps in modeling capabilities discussed. Potential applications are also discussed, describing how probabilistic predictive models could be used for a more agile LPBF qualification workflow.

This work was supported by the LDRD program at SNL, managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Advances in discretization techniques, element technology, mesh adaptivity, and solution strategies for inelasticity, localization, and failure

July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A FUNDAMENTALLY NEW COUPLED APPROACH TO CONTACT MECHANICS VIA THE DIRICHLET-NEUMANN SCHWARZ ALTERNATING METHOD

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ABSTRACT

Contact phenomena are essential in understanding the behavior of mechanical systems. Existing computational approaches for simulating mechanical contact often encounter numerical issues, such as inaccurate physical predictions, energy conservation errors, and unwanted oscillations. We introduce an alternative technique, rooted in the non-overlapping Schwarz alternating method, originally developed for domain decomposition. In multi-body contact scenarios, this method treats each body as a separate, non-overlapping domain and prevents interpenetration using an alternating Dirichlet-Neumann iterative process. This approach has a strong theoretical foundation, eliminates the need for contact constraints, and offers flexibility, making it well-suited for multiscale and multiphysics applications.

We conducted a numerical comparison between the Schwarz method and traditional methods like Lagrange multiplier and penalty methods, focusing on a benchmark impact problem. Our results indicate that the Schwarz alternating method surpasses traditional methods in several key areas: it provides more accurate predictions for various measurable quantities and demonstrates exceptional energy conservation capabilities. To address the issue of unwanted oscillations in contact velocities and forces, we explored various algorithms and stabilization techniques, ultimately opting for the naïve-stabilized Newmark scheme for its simplicity and effectiveness. Furthermore, we validated the efficiency of the Schwarz method in a three-dimensional impact problem, highlighting its innate capacity to accommodate different mesh topologies, time integration schemes, and time steps for each interacting body.

Constitutive modeling of complex materials with machine learning and artificial intelligence
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NOVEL METRICS FOR ASSESSING THE QUALITY AND COMPLETENESS OF STRESS-STRAIN DATASETS: BRIDGING THE GAP IN CONSTITUTIVE LAW DEVELOPMENT

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ABSTRACT

The accurate characterization of stress-strain datasets is crucial for developing robust constitutive laws for materials, essential in engineering applications. This paper introduces metrics to evaluate dataset quality and completeness, aiming for effective utilization in law development. Multiple stress-strain datasets, generated under random loading conditions, are considered, covering various material properties via the J2 constitutive law. Metrics are calculated for these datasets, and a deep neural network learns patterns within the data. The study focuses on evaluating metric accuracy by benchmarking against stress-strain datapoints collected from Finite Element Method (FEM) macro problems, for which the same metrics are also calculated. Comparing metric similarity between the benchmark problem and generated datasets, the best metric exhibits higher similarity, resulting in lower error in predicting stress-strain datapoints. In other words, the best metrics effectively capture knowledge, enriching the training database. This research establishes a standardized framework for assessing stress-strain datasets and enhances reliability in data-driven constitutive law development. The findings advance materials science and engineering practices, promoting a more systematic approach to material behavior analysis.

Multiphysics and data-driven modeling for cardiovascular biomedicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SIMULATION OF THE HEART USING NNFE

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ABSTRACT

With advances in computational modeling and imaging techniques, patient-specific cardiovascular modeling for device design, disease modeling and treatment is approaching reality. However, the slow computational speed for accurately simulating the complex physiology of the heart using traditional finite-element based methods still limits their practical clinical applications. While reduced order models are used to accelerate simulations in many domains, the time savings are insufficient and can include loss of accuracy.

We have previously demonstrated the efficacy of the neural network finite element (NNFE) approach for predicting cardiac mechanics of an idealized left ventricle within clinically relevant timeframes without compromising accuracy. In the present study, we extended the NNFE approach to a realistic ovine heart left ventricle (LV) geometry to simulate the pressure-volume (P-V) active contractile behavior over the complete functional range. The finite element mesh was created from MRI scans and principal myofiber directions were prescribed using DT-MRI data, all obtained from a single ovine heart. We modeled the constitutive behavior of the myocardium using a Fung-based hyperelastic material model, and the active contraction using an additive stress based on the Hunter-McCulloch-Ter Keurs model. The NNFE approach uses neural networks (NNs) to represent the discretized displacement field, and conventional finite elements to map the NN output on the problem domain, as well as to specify the boundary conditions and perform numerical integrations. The NN was trained with a physics-based training scheme using variational principles that minimize the norm of residual force vectors. Consequentially, this approach does not rely on the existence of a potential energy formulation of the boundary value problem (BVP), and extends the NNFE approach to capture non-conservative BVPs.

The NNFE model predicted the displacement field for any P-V loop in the physiological training space with a max nodal error <1%. The NNFE model took 2-5 hours for training, and once trained the NNFE model took ~3 seconds for producing results for any loading, whereas the traditional finite element (using Abaqus) model required ~2.5 hours on average for a single loading path. Our results demonstrate a major step forward in the application of the NNFE approach for organ level simuations. We are working on extending this method to study the effects of inotropy on cardiac behavior and disease simulations.

Advanced multiscale and adaptive numerical methods for non-linear solids
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HYBRID HIGH-ORDER METHODS FOR TIME-DEPENDENT, COUPLED ELASTO-ACOUSTIC WAVE PROPAGATION

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ABSTRACT

Owing to the complexity of geological features, the simulation of elasto-acoustic wave propagation in the Earth, is challenging. To handle efficiently this difficulty, we consider hybrid high-order (HHO) methods, which offer several attractive assets such as local conservativity, geometric flexibility through the support of polyhedral grids, and high-order precision [Di Pietro, Ern, 2014, Comput. Meth. Appl. Mech. Engrg.]. HHO methods rely on a pair of unknowns, combining polynomials attached to the mesh faces and the mesh cells. The cell unknowns can be eliminated locally using a static condensation procedure, whence an increased computational efficiency with respect to classical DG methods. HHO methods are closely related to hybridizable DG (HDG) methods [Cockburn, Gopalakrishnan, Lazarov, 2009, SINUM]. Here, we build upon previous work on HHO methods for either elastic or acoustic wave propagation in the time domain [Burman, Duran, Ern, 2022, Comm App Math Comp Sci], and devise the coupling between both HHO discretizations. A first-order formulation in time is considered, and implicit and explicit Runge--Kutta schemes are used for the time discretization. An energy balance confirming the stability of the schemes is derived. Numerical results on test cases with analytical and semi-analytical solutions show that the methods deliver optimal convergence rates. A more realistic case on the propagation of an elastic pulse in a sedimentary basin coupled to the atmosphere is presented. In accordance with what is observed in practice, we show that in such a case a significant part of the energy is captured by the sedimentary basin and then transmitted to the atmosphere.

Continuum biomechanics of active systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PATIENT-SPECIFIC SURROGATE MODEL TO PREDICT PELVIC FLOOR STRETCH DURING VAGINAL DELIVERY

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ABSTRACT

Between 6% and 40% of vaginal births may result in trauma to the pelvic floor muscles (PFM), leading to long-term consequences such as incontinence or prolapse [1]. Computational simulations can be used to biomechanically analyze the birth process; however, the integration of these simulations into clinical practice is hindered by high computational costs. To overcome this limitation, surrogate models can replace the simulations, enabling faster results. This study aims to develop an AI framework for predicting PFM stretch during vaginal delivery.

A finite element model of the PFM and fetal head was used to simulate delivery. Material properties and muscle geometry were varied to achieve patient-specific characteristics. A dataset of 5618 completed simulations was generated, with each pelvic floor node corresponding to an observation. Specifically, 49 nodes were selected near the urogenital hiatus of the PFM. The study used initial node coordinates, material properties, muscle diameters, node position, urogenital hiatus length, and time frame as training features. Decision trees (DT), random forest (RF), extreme gradient boosting (XGBT), and artificial neural networks (ANN) were selected as machine learning models. A 90/10 split was used to generate training and test sets, with the stratified shuffle split method ensuring a consistent feature distribution. Hyperparameter optimization with cross-validation was performed, and model performance was evaluated using mean absolute error (MAE).

The stretch was predicted for multiple instants of fetal descent to determine both its peak and the instant when it occurs. Preliminary results included a MAE of 0.239 mm for the DT model, 0.200 mm for the RF model, 0.544 mm for the XGBT model, and 0.397 mm for the ANN. By specifically analyzing the results obtained at each time step and node region, it was concluded that errors are higher for time steps closer to the end of the delivery and in the middle region of the muscle (corresponding to the region experiencing greater stretch).

The development of this framework consists of a preliminary step toward the implementation of patient-specific, near real-time computational simulations in a clinical setting. The ability to predict the stretch suffered on the pelvic floor immediately before or during childbirth could aid in medical decision making and in the identification of non-visible injuries.

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Analytical models for nonlinear dynamics and evolved dynamics in natural, social and engineering sciences
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATION OF THE HARMONIC BALANCE METHOD TO PREDICT WAVE PROPAGATION IN ONE-DIMENSIONAL NONLINEAR METAMATERIAL EXCITED HARMONICALLY

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ABSTRACT

Periodicity and local resonance are features managed to achieve efficient metamaterials. In the vast majority, the latter aspect is studied through the application of linear resonators. Recently, due to dynamic characteristics provided by nonlinearity, such as the dependence of the response on the amplitude of the excitation and the transfer of wave energy to higher harmonics, nonlinear resonators have been considered.

Nonlinear behavior is typically a challenging aspect to address. It often increases complexity and must be carefully analyzed at the design stage to avoid trial-and-error approaches in the design of mechanical devices.

This requirement is pursued in this work, where the objective is to develop a computational procedure capable of capturing some nonlinear behaviors in a one-dimensional metamaterial chain, such as the emergence of higher harmonics in the response and the influence of excitation amplitude. For this purpose, the Harmonic Balance Method (HBM) is implemented with a numerical continuation, considering the steps of pseudo arc-length and Newton methods.

The implementation of the HBM method is validated for a 2-DOF system with nonlinear cubic stiffness. Subsequently, a system with 10 unit cells is analyzed, each cell composed of a main chain mass connected to a local oscillator by a nonlinear cubic spring, a linear spring, and a viscous damper. Between consecutive unit cells, there is a linear spring and a viscous damper.

By applying a harmonic force to the first unit cell, the aim is to observe the vibration transmissibility throughout the structure. By observing the harmonics that compose the response, it is possible to evaluate the energy transfer to higher harmonics and the excitation force effect due to nonlinear dependency. The results and analysis can motivate new procedures for the design of metamaterials.

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Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A DISPLACEMENT-BASED MATERIAL POINT METHOD FOR WEAKLY COMPRESSIBLE FREE-SURFACE FLOWS

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ABSTRACT

We present a displacement-based material point method for simulating weakly compressible free-surface flows and fluid-structure interaction. To address volumetric locking, we employ the F-bar technique, previously developed for solid mechanics. This technique involves projecting the pressure and the dilatational part of the velocity gradient onto a lower-dimensional approximation space, eliminating complexities associated with two-field mixed formulations and operator splitting approaches. Additionally, to mitigate spurious pressure oscillations resulting from the use of a density-dependent equation of state, we enhance the framework with an artificial viscosity term. Finally, we employ higher-order spline background shape functions, resulting in a continuous representation of the velocity gradient and effectively preventing pressure jumps when material points cross element boundaries. Challenging numerical examples are provided to verify and validate our approach, demonstrating results that closely align with existing literature, exhibit reduced pressure oscillations, and are free of volumetric locking issues.

Physical models and reduced order models augmentation with data for physics-informed machine learning in real-world applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

UNVEILING BISTABLE STOCHASTIC DYNAMICS THROUGH PHYSICS-INFUSED LEARNING IN SCARCE AND NOISY DATA REGIMES

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ABSTRACT

Data assimilation and accurate identification and estimation of parameters in bistable stochastic systems pose significant hurdles. Traditional assimilation methods may struggle to capture the coexistence of multiple stable solutions and may fail to capture intricate nonlinear interactions within the system. In particular, applications such as energy harvesting, which involve mechanoelectric coupling, introduce additional complexities because of the interplay between mechanical and electrical components. On top of that, in real-world scenarios, obtaining observations for bistable systems might be limited and noisy. The scarcity of reliable data can hinder assimilation methods that heavily rely on observational information for accurate state estimation.

In response, we propose the use of deep learning for the characterization of bistable energy harvesters. The approach of Callaham et al. [1] will be complemented by the use of a penalty based on the fulfillment of the Fokker-Planck equation. The goal of this additional constraint is to combine the available noisy data with the knowledge of the system to fill the gaps of the unknowns in each separate framework and enrich the method.

Gaussian Process Latent Force Models (GPLFM) extend the concept of Gaussian processes (GPs) to include latent forces acting on the observed data. This approach is commonly used in machine learning and statistical modeling to capture complex relationships and dynamics in data, particularly in scenarios where forces or latent variables influence the observed outcomes [2]. Provided the stochastic nature of the loads triggering the dynamics of energy harvesters, this framework is used to formulate the latent forces as Gaussian Processes.

The combination of machine learning and physics-informed constraints enhances the robustness and interpretability of sensor and load characterization in complex systems with small and noisy datasets. The approach yields the reconstruction of the response surface of the dynamics under study, allowing the exploration of parameter combinations. Furthermore, an update algorithm is developed for the hybrid twin of individual energy harvesters, facilitating the continuous characterization of the mechanical properties and the stochastic load.

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Machine learning and multiscale modeling for complex materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RETHINKING GENERATIVE INVERSE DESIGN: A GENERAL AND LIGHT-WEIGHT MACHINE LEARNING FRAMEWORK FOR ON-DEMAND NONLINEAR MATERIALS DESIGN

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ABSTRACT

Data-driven engineered materials design offers prospects for developing structures and systems with evolutionary material properties. In contrast to forward modeling, the inverse design process is challenging due to its intractability and non-uniqueness of potential solutions. Current data-driven inverse design methods mainly employ deep learning, which has high data demand and requires expensive training and hyperparameter tuning. In this work, we propose a light-weight, single-shot inverse design method that generates engineered materials designs with target nonlinear constitutive relations, founded on statistical inference and Markov chain Monte Carlo (MCMC) sampling. Specifically, given any machine learning model that predicts materials' nonlinear constitutive relation and its uncertainty, we can estimate the likelihood of any possible material design satisfying any given target constitutive relation. We can then sample new material designs based on the estimated likelihood. Thus, the proposed method operates as a generative model for design solutions, capturing the one-to-many relationship between the target and designs and characterizing the distribution of acceptable outcomes based on a specified design target. The method also decouples the inverse design process from the forward modeling process, leading to enhanced customizability and universality. The inverse design process does not involve model training and hence is cost-efficient. The explicit likelihood estimation indicates the probability of target satisfaction and adds interpretability to the inverse design process. We validate the performance of the proposed method on a nacre-inspired metamaterials design problem. Subsequent experiments using synthetic design data further demonstrate the method's effectiveness, providing more detailed and visually represented quantitative functional behavioral results. This work presented an alternative view to solving on-demand inverse design problems through a less data and computationally intensive approach, and laid the foundation for future advancements in engineered materials design.

Multi-scale, multi-rate damage and fracture: Models, experiments, and simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PYMESOSCALE: A FRIENDLY PYTHON LIBRARY FOR GENERATING 3D CONCRETE MESOSCALE MODELS BASED ON THE LOCAL BACKGROUND GRID METHOD

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ABSTRACT

Mesoscale modelling of concrete and its composites has attracted a lot of researchers over the years with the promise of establishing an accurate relationship between the mesoscopic model and the macroscopic mechanical properties of concrete. The main issues preventing such outcomes are (1) difficulty in generating a high aggregate volume fraction with control over aggregate shape and gradation. (2) computational resource consumed when generating mesoscale models, (3) realistic ITZ (Interfacial Transition Zone), (4) effective aggregate intrusion detection when placing aggregates etc. But among these issues, lies a much bigger one which is the lack of open sourcing of codes and algorithms that were implemented in research papers slowing down the speed at which research would have progressed. Researchers have to program the algorithms of previous research in order to improve or devise newer and more effective ones. Comparison between the newly developed and already existing mesoscale model generation algorithm will require programming, slowing down the pace by which important problems can be solved. Moreover, most papers do not give a complete overview of the most delicate and subtle details required to implement such algorithms leading to reading multiple papers for the implementation of a single algorithm [1,2]

pyMesoscale implements the local background method for generating 3D mesoscale models which have proved to be amongst the most effective mesoscale generation algorithm particularly with a much better aggregate intrusion detection system during aggregate placing and a high aggregate volume fraction after packing. The generated aggregates are randomly translated onto a global mesh where all the elements have been initialized as mortar. A local background grid is generated around the translated aggregate where all aggregate and ITZ identification and intrusion takes place. Python was the programming language of choice due to its smoother learning curve and beginner friendliness. Reducing implementation complexity was at the heart of its development making it approachable by both new and experience researchers to the field. Sufficient documentation in the form of Docstrings (Documentation String) have been written for easy and fast reference to users of the library. More mesoscale model generation algorithms will be added in newer versions of the library giving researchers the ability to compare and contrast between algorithms.

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Multiphysics and data-driven modeling for cardiovascular biomedicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A TWO-WAY COUPLING FRAMEWORK FOR IMMERSED HETEROGENEOUS STRUCTURES IN FLOW WITH APPLICATIONS IN VASCULAR SYSTEMS

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ABSTRACT

Immersed heterogeneous structures are prevalent in various engineering and biological applications. Examples include flow and nutrient transport into and around porous corals [1]. Within the vascular system, the blockage and fracturing of porous blood clots under pulsatile flow [2] is driven by clot-flow two-way interactions. These problems are characterized by a soft, discrete heterogeneous structure deforming under unsteady viscous flow-induced forces. Numerical simulations of the inherently multi-scale flow and flow-structure interactions of such complex structures pose a significant challenge. Using mesh conforming fluid-structure interaction methods can result in highly distorted mesh elements when structural deformation is large. Non-conforming methods such as the Immersed Finite Element Method (IFEM) [3] provide an attractive avenue for simulating an immersed continuous structure without expensive re-meshing. However, a continuum-based representation of the heterogeneous structures does not capture the inherently discrete micromechanics effectively. Additionally, modeling discontinuous phenomena, such as fracture (referred to as clot embolization), is not straightforward using a continuum-based representation. Here, we describe a method that extends IFEM by representing the structure as a series of connected mesoscopic discrete elements. Utilizing a discrete element representation allows for the direct representation of the structure's discrete properties, such as porosity, and enables modeling of discontinuous phenomena like fractures. Dynamics of the discrete elements are solved through a customized Discrete Element Method (DEM) framework. Fluid-structure interactions from each discrete element and the internal forces arising from discrete element interactions are coupled back into the background fluid flow using underlying elements of the IFEM framework. This results in a two-way coupled fluid-structure interaction framework for an immersed discrete structure. To validate the inter-element interaction aspect of the implementation, we present results from a canonical immersed two-body problem simulated using our framework. Furthermore, we compare an example problem of an immersed heterogeneous structure with an existing immersed continuous structure counterpart. Finally, we demonstrate an example application of our method by simulating the micromechanics of a porous blood clot under pulsatile flow.

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OPTIMIZATION OF FUNCTIONALLY GRADED POROUS ACETABULAR COMPONENT

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ABSTRACT

Introduction: The mismatch of stiffness between the host bone and the stiffer acetabular components (made of ceramic or metallic alloy) causes stress/strain shielding, leading to peri-prosthetic bone resorption and eventual mechanical loosening. The functionally graded porous (FGP) design capitalizes on the benefits of porosity while maintaining mechanical strength, suggesting its superiority over the uniformly porous counterparts. Although a porous implant facilitates better tissue ingrowth, the reduced stiffness might result in higher volumetric wear of the polyethylene (PE) liner. The objective of the study was to determine the optimal design parameters of the functionally graded porous acetabular component that would result in a trade-off between volumetric wear of the PE liner and bone resorption.

Methods: The elastic properties of the porous metal-backing were determined using a numerical homogenization of the octet-truss unit cell. The multi-objective optimization problem (MOOP) was solved using a non-dominated sorting genetic algorithm. The percentage of resorbed bone mass fraction and the volumetric wear were considered as the objective functions. Porosity levels (porosity values at acetabular rim, and dome) and functional gradation exponents (radial and polar) were considered as the design parameters. The optimal functionally graded porous designs (OFGPs) 1-5 were obtained after employing a simple ranking method named Technique for Order Preference by Similarity to Ideal Solution analysis (TOPSIS) on the Pareto-optimal solutions. The sensitivity of different design parameters of FGP metal-backing on the objective functions were evaluated using multivariate analysis.

Results: The OFGP-1, having highly porous acetabular rim and less porous dome, exhibited a superior trade-off between the bone resorption and the volumetric wear of the PE liner across all OFGPs. More bone elements (~75%) were subjected to higher strains (1.1 - 1.5%) for the OFGP-1 as compared to those for the solid metal-backing. However, OFGPs exhibited an increase in volumetric wear (3-10%) compared to solid metal-backing. Based on the multivariate analysis, it was found that the objective functions were more sensitive to changes in the values of polar gradation exponent ($m\theta$) as compared to that of radial gradation exponent (mR). Statistical analysis indicated that the bone resorption and the volumetric wear of the PE liner were most sensitive to the porosity limit at the inner rim and the porosity limit at the dome, respectively.

Conclusion: The OFGP-1 appeared to be a viable alternative to the solid metal-backing. The results also indicated the superior performance of the OFGP-1 over the uniformly porous design (OFGP-5).

Fracture, damage and failure mechanics of cementitious materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELACIÓN DE RÓTULAS PLÁSTICAS EN ELEMENTOS ESTRUCTURALES DE CONCRETO REFORZADO - REFORZADO- MODELING OF PLASTIC HINGES IN REINFORCED CONCRETE STRUCTURAL ELEMENTS

Marlyn Arantza Muñoz Moscoso[*1], Jairo Andres Paredes Lopéz*[1] *and Daniel Bedoya-Ruíz*[1]

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ABSTRACT

The significance of studying the behavior of plastic hinges in reinforced concrete structural elements arises from the desire to comprehend how structural design computer programs implement structural analysis in the nonlinear or deformation range, with the goal of maximizing structural integrity. However, these results remain highly generalized to the structure, prompting a deeper investigation into the stress and deformation characteristics of composite materials, such as the well-known combination of steel and concrete. Additionally, plastic hinges serve as "devices" for dissipating energy, particularly during events like earthquakes. This mechanism allows for controlled plastic deformation at the connection of a column, effectively absorbing energy.

In contemporary seismic resistant design studies, the focus has been on developing new technologies for novel constructions. Regrettably, conventional structures, which constitute the majority of Colombia's built environment, have been somewhat neglected. This underscores the necessity of probing the behavior of structures holistically, deconstructing them into finite elements possessing easily analyzable mechanical characteristics. This approach facilitates the identification of failure points, validation of plastic hinge theories, and examination of prevailing design procedures. It's important to rectify situations where creativity sometimes leads to overly rigid structures with excessive angularity, often resulting in unanticipated torsion.

To model joint development, beam-column finite elements with interior discontinuities are formulated. These elements account for damage by simulating the emergence of cracks, transverse displacements, and axial irregularities. Employing constitutive models rooted in damage mechanics and drawing from experimental tests detailed in existing literature, these finite elements encompass moment capacity, shear force, and axial force considerations, encompassing the behavior of concrete reinforced with steel. Numerical instances of reinforced concrete beams and frames subjected to damage-inducing loads are presented to illustrate the damage modeling capabilities of the developed finite elements. The load-displacement curves calculated in these numerical examples exhibit consistency with those documented in literature.

Consequently, this investigation aims to analyze the behavior of plastic hinges within a reinforced concrete portico, comprising beams and columns. Through numerical analysis, we delve into the mechanical behavior of these elements and draw comparisons with current regulations. Nonlinear analysis employs the finite element method as a computational tool, leveraging series/parallel mixture theory. Constitutive models that accurately represent the mechanical properties of each material underlie the nonlinear numerical analysis.

Computational fluid dynamics (CFD) and fluid-structure interaction (CFSI): Methods and Applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CFD STUDY OF PARTIAL POROUS COATING TO ENHANCE AEROACOUSTICS IN BLUFF BODIES

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ABSTRACT

Flow control for bluff bodies has been object of attention for many researchers for a long time. Particularly, the study of cylinders in different configurations, as they might appear in the geometry of the pantograph of a high-speed train, has been considered in [1]. The increase of train speed has resulted into a larger fluctuating contact force between the pantograph and the catenary, introducing instabilities in current collection. Nevertheless, a more significant problem in pantographs is the associated aerodynamic noise, which becomes significant at train speeds over 300 km/h. To reduce the Aeolian tones, flow control has been proposed. Among the different passive flow control techniques, covering with porous material has been applied in [2]. However, the enhancement of the aeroacoustics by this approach has also meant an increase of the drag coefficient. Besides, typically this has been studied coating the whole side of the cylinder. Only in [3] a partial covering was considered, concluding that coating 1/4 of the cylinder surface, around the detachment point, might be a good a compromise between improving the aeroacoustics and reducing the amount of porous material to be used. Here, a more complete parametric study of the position of this partial coating is proposed, ranging from 15 to 180 deg. of symmetric coating (from the stagnation point). A CFD analysis using Scale-Adaptive Simulation (SAS) turbulence model has been completed, and the results obtained show how covering the first 30 deg. let reducing both drag and fluctuation of lift coefficients, as well as sound pressure level.

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Topology optimization for additively manufactured metamaterials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STUDY OF OBJECTIVE FUNCTIONAL IN OPTIMAL DESIGN OF PHONONIC CRYSTALS FOCUSING ON BAND GAP IN HIGH FREQUENCY RANGE

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ABSTRACT

Phononic crystals exhibit unusual dispersion properties such as band gap where elastic waves can not propagate to any direction because of interference or local resonance. As an attempt to take advantage of the dispersion properties of phononic crystals, vibration suppression and waveguide applications are underway, and studies on controlling heat conduction on a microscopic scale have begun. Since dispersion properties of phononic crystals depends on shape, scale, and material of the structure, effective design method is essential for the applications. Topology optimization method is studied as the design method and shown to be able to design phononic crystals with desired dispersion properties. Maximization of band gap width has been one of the most addressed cases as a benchmark. However, formulations that have been used in previous studies have difficulty optimizing the band gap in high-frequency bands where multiple modes are dense. Consideration of dispersion properties in the high-frequency band is important in the application of phononic crystals on the microscale. In this study, we propose an objective function to create and maximize the band gap in the high-frequency band and verify its effectiveness. Additionally, in the formulation of the optimization problem, connectivity of the structure and how to deal with localized modes are also be discussed.

PSE (Problem Solving Environment)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

YOGA THERAPEUTIC APPROACHES FOR THE PHYSICAL AND MENTAL HEALTH OF OLDER ADULTS: USING MOVEMENT ANALYSIS AND PSYCHOMETRIC DATA ANALYSIS

Satoko Murakami[*1], Chieko Kato[1] and Hongjie Zheng[1]*

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ABSTRACT

Background: Enhancing the healthy life expectancy of older adults and meeting their needs, such as purpose in life, not only helps to keep them physically and mentally healthy and improve their quality of life in their later years but also encourages active social participation and promotes the overall development and inclusiveness of the society. Objectives: Although various therapies for older adults have been proposed, the effects of yoga therapy on the physical and mental health of older adults have received extra attention. Therefore, this study was conducted to clarify the effects of yoga therapy on older adults' physical and mental health, which was verified by combining psychological data and movement analysis. Methods: A healthy older adult served as a tested participant in this study and was subjected to six yoga therapy sessions once a week with gymnastics and breathing exercises in chair yoga therapy. Yatabe-Guilford Personality Test (YG Test) and POMS-2 short version (Profile of Mood States Second Edition) were performed at the beginning and the end of the yoga therapies for before and after comparisons. In addition, we filmed the yoga therapy practice with a video camera, detected the posture of shoulder rotation movements in contact with Open Pose, and put the CSV data in chronological order. Moreover, psychometric test results and interviews about impressions of yoga therapy were included in the different studies. Results: During the first to sixth sessions, the range of motion of the shoulders, elbows, and wrists increased. In the YG test, there was an increase in scores for generally active activities; in the POMS test, there was a decrease in scores for anxiety and depression and an increase in scores for vigor. Conclusions: The possibility of visualizing yoga therapeutic movements to clarify their relevance to psychological aspects will be pursued. It is essential to consider the perspectives of older adults when considering lifelong education.

Quantum scientific computing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

QUANTUM ANNEALING-BASED APPROACH FOR FLUID DYNAMICS SIMULATION USING FINITE ELEMENT METHOD AND TOPOLOGY OPTIMIZATION

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ABSTRACT

The Finite Element Method (FEM) is a numerical method for finding approximate solutions to differential equations and is widely used in engineering. Although FEM is useful for modelling complex systems, solving very large systems is computationally demanding and requires new approaches using promising techniques such as quantum computing. With this in mind, several quantum algorithms for FEM have been demonstrated. Examples include algorithms with theoretical speed-up guarantees using fault-tolerant gated quantum computers [1] and heuristic design optimisation algorithms using quantum annealing machines [2].

In this study, a framework for FEM with quantum annealing is presented with a focus on fluid dynamics problems. In this framework, the discretised equations of FEM are mapped to a quadratic unconstrained binary optimization (QUBO) problem, which can be solved by quantum annealing. The performance of the proposed method is numerically demonstrated on a simple two-dimensional potential flow.

Furthermore, we propose QUBO to optimize the solid-fluid topology of the fluid channel on the basis of the level-set idea [3]. The combination of the proposed QUBO and classical FEM fluid analysis is used to optimize the fluid channel topology with quantum annealing.

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PREDICTION OF PLURAL CRACK PROPAGATION USING DISCOVERED PDE

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ABSTRACT

This study presents plural crack propagation prediction using partial differential equation by equation discovery. Fatigue crack growth is simulated by numerical computations considering governing laws and fracture mechanics criteria: stress intensity factor, Paris' law, and criterion of crack propagation direction. It takes much time to compute a single crack propagation case using the finite element method. In contrast, machine learning can predict interpolated crack propagation path and its rate in a much shorter time than the finite element analysis. Therefore, machine learning can efficiently evaluate a structure's integrity on a site.

A dataset is obtained from the results of crack propagation analyses using s-version FEM (s-FEM) combined with an automatic mesh generation technique. Crack propagation can be predicted by machine learning with appropriate input data design. The input parameters are coordinates of the 4 crack tips, the output data are crack propagation vectors, and the number of crack propagation cycles of 0.25 mm. Firstly, the coordinates of each crack tip are given to the predictor. Secondly, the propagation rate and direction are predicted by machine learning. Finally, the next crack coordinate is calculated. A series of these procedures are iterated to predict the crack propagation. The loss is defined by the weighted sum of the prediction loss and the partial equation loss. The definition of two losses is called as physics informed neural networks. The advantage of the loss definition is accelerating of train. PDEs are discovered by evolutionary algorithms. The PDE are composed by 1st and 2nd order partial derivatives of the input and output parameters. It is expected that the loss of PDE as regularization will accelerate training, improve prediction accuracy and minimize loss more rapidly.

The important thing is that the PDE, which can be minimized with less iterations of training, should be appropriately specified using an equation discovery technique. We'd like to discuss how machine learning can be applied to actual engineering problems to generate accurate predictions with less iterations.

Imaging-based methods in computational medicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INFERRING MECHANICAL PROPERTIES OF TISSUE WITH QUANTIFIED UNCERTAINTY USING CONDITIONAL GENERATIVE MODELS

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ABSTRACT

Elasticity imaging involves probing the deformation of tissue non-invasively using a standard imaging technique like ultrasound, magnetic resonance imaging, or optical coherence tomography. This yields a noisy and incomplete measurement of the deformation field inside the tissue in response to an excitation. The goal is to use this deformation field and the knowledge of the physics of deformation to determine the spatial distribution of its mechanical properties. This is a challenging and ill-posed inverse problem where prior information about the tissue plays a significant role. In this talk, we will describe the use of conditional generative models to solve this problem in a probabilistic setting. This approach provides us with an estimate of the tissue properties as well as the uncertainty associated with this estimate. Applications include imaging the mechanical properties of the inner eye and that of tumor spheroids growing in a soft medium.

MULTISCALE TOPOLOGY OPTIMISATION FOR NONLINEAR ELASTIC STRUCTURES

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ABSTRACT

In this presentation, a multiscale structural optimization framework capable of efficiently designing two-scale structures with prescribed displacements in the nonlinear elastic regime is presented. In contrast to previous multiscale structural optimization frameworks, which are founded upon the assumptions of linear elasticity, the present framework is capable of efficiently operating within the nonlinear elastic regime. At the core of the present framework is a parameterized microscale geometry (or metamaterial), which through the straightforward manipulation of the microscale parameters provides direct access to both positive and negative Poisson's ratios. The microscale model is concurrently coupled to the macroscale model, such that only the microscale parameter space traversed by the optimizer is resolved during the optimization procedure, leading to a significant reduction in the computational expense of analysis. To demonstrate the capability of this framework, two prescribed deformation profiles are targeted by two distinct optimization procedures. In both instances, the deformation profile is successfully targeted. To verify the accuracy of the optimized structures, high-fidelity single-scale simulations are performed. In each case, excellent agreement is noted between the high-fidelity simulations and the corresponding optimized macroscale displacement fields, with errors of less than 10\%.

Mesh-free particle methods for multi-physics problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ASSESSMENT OF MINING TAILINGS SPILL IMPACTS WITH THE WEAKLY COMPRESSIBLE MPS METHOD

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ABSTRACT

Accidents causing sudden failures of mining industry tailing dams and subsequent toxic material spills have been extensively documented. The consequences of such incidents pose long-term threats to surrounding environments and ecosystems. It is therefore crucial to develop effective models for assessing the potential impact of these flows and formulating comprehensive response and management plans. The initial release of tailings, being marked by significant deformation and fragmentation, poses a serious challenge to traditional mesh-based numerical methods. Moving particle semi-implicit model (MPS) due to its fully Lagrangian nature offers a unique opportunity to handle such complex physics and is flexible enough to accommodate their non-linear behaviors.

In this study, we employ a three-dimensional (3D) multiphase weakly compressible moving particle semi-implicit (MPS) model to simulate overland flows and evaluate the impact of the material spread within the area of interest. The model incorporates the enhanced represented polygons boundaries (ERP) instead of traditional ghost particles to accurately represent real topography, enabling large-scale applications. To address the non-linear behavior of tailings, Bingham plastic and Herschel-Bulkley rheologies are adopted. The model is applied to simulate the Brumadinho tailings and a hypothetical dam breach at the Copper Mountain tailings dam in British Columbia, anticipated to be the second largest after extension. Simulation scenarios include a single-flow mixture and a multiphase flow with a tailings pond capping the mixture. Numerical results demonstrate the capability of the method to capture the dynamic of the flow and both its scale and intensity with reasonable accuracy.

Contact and interface mechanics: Modeling and computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

POWER DISSIPATION MODELLING IN ROLLING CONTACT

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ABSTRACT

This paper deals with the estimation of power dissipation due to friction and simulation of the wear evolution in rolling contact problems including Coulomb rather than Hertz friction model as well as the frictional heat flow. The displacement and stress of the rail in contact are governed by the coupled elasto-plastic and heat conductive equations. We focus on power dissipation modelling rather than contact stresses as in [1]. This work develops new approach to estimate numerically power dissipation and wear modelling in wheel – rail contact problems and provides new insights into the research of these problems. The wear is computed for wheel – rail contact for elasto-plastic material model rather than elastic material model only. Wear estimation is based on combined power dissipation and Archard models rather than Archard model only [2,3].
Numerical model is solved using generalized Newton method rather than Fastsim or Contact software methods. The update finite element mesh algorithm related to the worn material volume rather than general type algorithm is used. The obtained numerical results indicate that the obtained contact patches are characterized by longer zones and lower stress intensity than in the elastic case. For relative small increase of temperature the contact patches are slightly longer than for plasto-elastic model. The power dissipated as well as the wear rate are strongly dependent on the friction coefficient, i.e. they increase when the friction coefficient increases.

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Geometric mechanics formulations and structure-preserving discretizations for continuum mechanics and kinetic models
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COADJOINT ORBITS FLUID IMPLICIT PARTICLES

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ABSTRACT

Incompressible fluids enjoy particle relabeling symmetry, giving rise to Kelvin's circulation conservation. Throughout the past two decades researchers have been actively developing methods that mimic this continuous property of fluids in the discretized simulations. From a computational fluid dynamics (CFD) viewpoint, these discrete models resemble finite difference or finite volume schemes, which unfortunately have limited stability conditions, despite alluring benefits of structure preservations. Thus non-structure-preserving (but more-stable) semi-Lagrangian, fluid-implicit-particle (FLIP), and particle-in-cell (PIC) schemes are still the dominating numerical methods in applied fluid simulations.

We propose a new approach to structure-preserving discrete fluids. This approach results in discrete models that resemble the mainstream FLIP or PIC methods, but with much more geometric structures.

By incorporating isogeometric analysis techniques (i.e. mimetic interpolation), a staggered grid velocity interpolates into a smooth divergence-free vector field. Furthermore, instead of only moving the positions of the particles by this interpolated velocity field, we let both the positions and the momenta be acted by this field in a symplectomorphic manner. This symplectomorphic group action therefore induces a momentum map, from the particles' position-momentum space to the dual space of velocities. We argue that this canonical map should be taken as the particle-to-grid information transfer. Since momentum maps are Poisson structure preserving, Hamiltonian flows of particles will map into a coadjoint orbit in the dual Lie algebra of divergence-free velocities. In particular, our method preserves Casimirs such as 2D enstrophy and 3D helicity.

Our method, named Coadjoint Orbits FLIP (CO-FLIP), undergoes the following transformation from the traditional FLIP method: The grid-to-particle transfer becomes a mimetic interpolation, the particle motion becomes a symplectomorphic action, and the particle-to-grid transfer becomes the momentum map. Each of these components are informed with each other. We showcase traditional simulation methods benefit from structure-preserving techniques by producing higher fidelity vortical structures, without the need of having prohibitively high resolution computation grids.

Advances in multi-scale, multi-material, and multi-component Topology Optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ON THE ACCELERATION OF A TWO-LEVEL TOPOLOGY OPTIMIZATION PROCESS FOR GENERATING QUASI-CONTINUOUS HIGH-RESOLUTION STRUCTURES

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ABSTRACT

ABSTRACT
Currently, Standard Topological Optimization tools are able to propose an optimal material distribution for the component, but when small topological details are required the computational cost becomes excessive. In order to overcome this drawback, the present work proposes a two-level topology optimization method in three main steps. The first one subdivides the whole component in cells and generates a coarse optimized low definition material distribution through the well-known SIMP method [1]. The second step uses an equilibrating technique [2] that provides tractions continuity between adjacent cells,. Finally, each cell is optimized at fine scale taking as input data the densities and the equilibrated tractions obtained from the coarse problem via the SIMP method again [3]. Thus quasi-ensuring the material inter-cell continuity after the cells optimization process.
Even if this 2-level approach allows to decrease the computational cost with respect to the full scale problem, the topology optimization processes at each cell, must be performed. Considering that each topology of a given cell could be parametrized with the input data (i.e. loads and density), an strategy based on the measurement of the distances in that parametric space is developed. This measurement is used in combination with a Machine-Learning tool to decrease the number of iterations in the topology optimization process in each cell by proposing a quasi-optimal initial topology in the optimization loop of each cell.

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Computational and analytical advances in nonlocal modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CUTTING-EDGE NODE-WISE CLASSIFICATION FOR AUTOMATED REGION IDENTIFICATION IN LOCAL AND NONLOCAL COUPLING MODELS

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ABSTRACT

Recent advances in mechanics focuses on coupling nonlocal models with classical local models. This coupling is motivated by the goal of reducing the high computational costs associated with high fidelity models like nonlocal equations, which are used in modeling and simulating complex material behaviors in materials science. Nonlocal models provide a more thorough depiction of certain phenomena that classical Partial Differential Equations (PDEs) cannot sufficiently represent. Such phenomena include the fractures and cracks [1]. In this context, various coupling methods, such as the Variable Horizon Coupling Method (VHCM) and matching displacements or stresses in overlapping regions, have been proposed [2]. This study introduces an innovative machine learning-based approach for automating the classification between local and nonlocal regions within the coupling process. This identification process takes various factors into account, including load functions, boundary conditions, and material geometry. The dataset includes diverse load conditions, such as loads with or without discontinuities. These loads are then preprocessed using the windowing approach, which proves highly effective in handling load functions with varying numbers of discontinuities and other conditions. This approach enables the examination of individual data points within the load. Utilizing window-based techniques, we formulate the problem as a node-wise classification approach. By applying window configurations around each data point, we segment the load effectively, facilitating a focused and precise classification strategy at each point. For the classification, we employ a Convolutional Neural Network (CNN)[3] as a deep learning algorithm that takes windows as input and assigns a label to the window's central node. The resulting output consists of labels assigned to central nodes, indicating either LM for the nodes located in the local region or NLM for the non-local region. The model exhibits exceptional performance, achieving an accuracy of 0.98 and an F1-score of 0.97. These results underscore the potential of our approach to significantly enhance coupling processes, leading to more accurate and computationally efficient designs in material science.

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APPLICATION OF XFEM USING CONTINUUM SHELL ELEMENTS TO DAMAGE PROPAGATION ANALYSES OF CFRP LAMINATE

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ABSTRACT

Due to high specific strength and stiffness, carbon fiber-reinforced plastics (CFRP) have been widely used in aviation industries in recent years. However, CFRP laminate is susceptible to out-of-plane load, leading to complex damage such as delamination, matrix crack, and fiber breakage. Because the damage may cause a decrease in compressive strength, CAI (Compression After Impact) strength is important in designing CFRP laminate structures.

This study applies an extended finite element method (XFEM) to damage propagation analyses of CFRP laminate. An eight-node quadrilateral interface element and an eight-node hexahedral continuum shell element enriched with only the Heaviside function are used to model delamination and matrix cracks, respectively. In addition, the zig-zag cohesive zone model is employed for delamination and matrix cracks to perform the implicit analysis successfully.

In this presentation, the implicit static method is used to perform damage propagation analyses of CFRP test specimens. It was shown that the proposed XFEM using continuum shell elements is an effective method for damage propagation analysis of CFRP laminates.

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Constitutive modeling of complex materials with machine learning and artificial intelligence
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MACHINE LEARNING APPROACH TO PREDICT IN VIVO SKIN GROWTH

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ABSTRACT

Skin growth through tissue expansion is an important process for many modern reconstructive surgeries including breast reconstructions and skin defect repair. When a tissue expander is inserted underneath the surface of the skin and inflated, the skin is held in a stretched position which triggers skin growth. Unfortunately, the procedure can have significant complications for patients, for example 8.9% of breast reconstruction patients have been reported to experience skin necrosis [1]. These complications are often the result of thin poor-quality skin and/or overexpansion.

Our previous research has shown that elastic wave measurements may be a suitable method for inferring in vivo skin tension [2]. As such, our goal is to use simulated data from a finite element (FE) model to train a machine learning (ML) model to determine in vivo material properties and predict future growth from measurements of elastic wave speed.

Abaqus was used to develop a 3D FE model to simulate in vivo human skin during the tissue expansion and wave propagation procedures. A custom user defined material was used to model the growth of the skin during tissue expansion [3].

The FE model was run for 1,000 unique sets of human-like material parameters sampled using a Latin hypercube technique. In each case, the skin material parameters, the growth field after 7 days and the waveform (displacement of a node 5mm from the origin of the surface wave) was stored. Using this dataset, an artificial neural network (ANN) was trained to predict growth and material properties.

The ANN was found to have excellent predictive performance for all target variables. The R2 value computed between the true FE outputs and the predicted ANN outputs were found to be 0.94 ± 0.03, 0.98 ± 0.06, 0.86 ± 0.03 and 0.98 ± 0.02 for the growth field, stiffness, growth rate and natural pre-stretch respectively.

Principal Contributions:

Currently, no method exists to non-invasively quantify in vivo skin growth. Thus, a model of the kind presented in this work, once validated, could result in a major advance for reconstructive surgeries. Surgeons could obtain non-invasive measurements of future growth, reducing overexpansion and complications for the patient. Furthermore, this framework could be used to explore different expander geometries/textures, subject specific inflation procedures etc.

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Industrial applications of IGA
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ISOGEOMETRIC CRASHWORTHINESS ANALYSIS: ADVANCES AND CHALLENGES

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ABSTRACT

In this talk we review recent developments of isogeometric analysis in LS-DYNA with particular focus on crashworthiness. We discuss the reason for and the importance of supporting a versatile set of geometric representations. Finally, we provide a glimpse into the latest industry trends and the challenges encountered as production-grade industrial deployment of the technology progresses.

THE “CHICKEN-EGG” ALGORITHM, A MULTIPHYSICS METHODOLOGY TO JACOBIAN TRIANGULARIZATION

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ABSTRACT

The role of non-dimensional ratios in engineering and physics is ubiquitous; but applied mathematicians sometimes overlook the utility of non-dimensional analysis. Notably, in the multiphysics modelling community, coupling methods are often discussed and developed without consulting the various non-dimensional ratios of the various inter-physics coupling terms. However, it is evident that the varying strengths of the coupling terms in a multiphysics model of N physics modules will influence either the convergence rate, the stability of the coupling scheme and the program execution speed. In fact, the analysis performed by Huang [1] explicitly showed that the “ordering” of the predictor physics modules is primordial to the performance characteristics of the multiphysics coupling scheme. However, the question of “how to order” (who came first, the chicken or the egg?) the N physics modules remains vaguely posed. In fact, physics ordering is generally based on the scientist’s experience or on problem specific stability analyses performed on academic computational configurations (see computational FSI and conjugate heat transfer literature). In the case of generic multiphysics coupling, where volume, interface and/or surface coupling terms can manifest, the optimal ordering of the physics modules may strongly vary along simulation time (for the same application) and/or across applications. Motivated to find an approximate measure that does not resort to cumbersome and problem specific stability analyses, we borrow the concept of non-dimensional analysis from physics and apply it to the algebraic systems that manifest in multiphysics computational models. The “chicken-egg” algorithm is based on a non-dimensional methodology that serves to “triangularize” the full Jacobian matrix of an exact Newton-Raphson implicit scheme. The method poses a non-dimensional preconditioner that estimates the different strengths of the various coupling terms found in the multiphysics application. The elimination of the small non-dimensional entries $\phi_{ij}<1$ and the row reordering of the preconditioner represents the now triangularized and “ordered” Jacobian of the multiphysics model. The “chicken-egg” algorithm estimates at every given time step the order of magnitude of ϕ_{ij} and correspondingly orders the N partitioned physics modules (automatically). This algorithm is tested for the first time on a thermo-hygro-corrosive multiphysics model and shows promising results. Compared to a classic sequential block-diagonal algorithm, the first numerical tests show over a 2-fold improvement in program calculation time.

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Data-driven methods for modeling complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CLUSTER-BASED CONTROL IN HIGH-DIMENSIONAL FLOW SYSTEMS THROUGH CONVOLUTIONAL AUTOENCODER

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ABSTRACT

We introduce an innovative architecture for cluster-based control of complex flows using high-dimensional data, addressing the limitations of traditional sensor-based methods. Traditional flow control strategies, whether model-free [1] or model-based [2], have relied on limited sensor measurements, leading to control laws that are often specific and lack generalizability across different features. We propose a novel methodology that fully leverages high-dimensional datasets to enhance control mechanisms. By employing a convolutional autoencoder, we compress the vast data into a manageable form, producing a low-dimensional embedding that captures the critical nonlinear dynamics of the system within latent space vectors. The subsequent clustering of the latent space informs a feedforward neural network, facilitating a direct mapping between the latent space vectors and key system quantities like the drag coefficient. This creates a clear interpretability of the clustered states, a significant advancement in understanding complex flow dynamics. We construct a cluster-based network model [3] to serve as a transition propagator between centroids in response to control inputs. This model informs the creation of a feedback control law that guides the latent space trajectory toward a desired cluster state. The control law is then decoded and applied as a forcing input, steering the high-dimensional system toward a targeted low drag state, particularly over an airfoil at a high angle of attack. The inherent speed and efficiency of our model stem from its foundation in low-dimensional latent space vectors, allowing it to encompass the full spectrum of high-dimensional system characteristics. Notably, the model demonstrates versatility, controlling multiple attributes simultaneously without extensive reconfiguration. This architecture signifies a leap forward in flow control, marrying full data utilization with rapid operational capability. It promises to reshape the way we approach control laws for complex systems, with potential applications extending beyond aerodynamics into various fields where flow dynamics play a crucial role.

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Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MATERIAL POINT METHOD MODELING OF CRACK PROPAGATION FOR INTERACTING AND INTERSECTING EXPLICIT CRACKS

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ABSTRACT

Numerical crack propagation modeling of multiple, explicit cracks requires methods that can resolve interacting, and potentially intersecting, cracks as well as methods to calculate crack-tip parameters with sufficient accuracy for predicting when and where cracks will grow. The material point method (MPM) can solve interacting crack problems using the CRAMP method (for cracks in MPM), but J integral calculations needed to predict crack propagation have to be modified whenever other cracks intersect the J contour for the propagating crack. If the tip of an intersecting crack is inside the J contour, the contour has to be adapted to avoid that tip. This talks will describe robust J calculations for interacting and intersecting cracks. Several examples show that the revised J methods are accurate even when J contours are intersected. Selected crack propagation examples show the new methods have sufficient accuracy for interacting crack propagation calculations. The calculations work with a regular background MPM grid without any need to remesh or to highly refine crack-tip regions.

Emerging topology and shape optimization techniques in computational design of materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE STRUCTURAL OPTIMIZATION USING MACHINE LEARNING SURROGATE MODELS FOR SECOND-ORDER HOMOGENIZATION

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ABSTRACT

Multiscale structural optimization considers the simultaneous design of both the macroscale (observable) structure and its microscale constituents. In this work, microstructures with intricate features are used to control local structural properties. Driven by advancements in additive manufacturing, the introduction of complicated microarchitectures in the microscale design space can produce superior structures for high strength-to-weight and energy absorption applications. Numerical homogenization techniques that have traditionally been used to incorporate microarchitecture mechanics into multiscale design, however, fail to capture local physical phenomena. The deliberate integration of these microarchitectures into the greater structure must also include both microscale and macroscale design variables. To address these challenges, numerical homogenization is typically used to estimate the local response of the microarchitecture, while design parameterization is used to limit the multiscale design space.

This presentation seeks to extend the homogenization approach to design using machine learning. As in traditional topology optimization, we implement a surrogate for parameterized homogenization to model the micro-to-macro transition. As a surrogate, we explore the deep neural network (DNN) for its ability to efficiently model high-dimensional and nonlinear functions. In addition, we build the DNN's training dataset using finite element simulations of second-order numerical homogenization. The second-order homogenization method incorporates a strain gradient into the microstructural analysis, increasing the information exchange between the macro- and microscales and addressing problems of scale separation. The model is applied to evaluate the local stress amplification caused by spatially varying microarchitectures. Through numerous examples, we show how a model can be used to efficiently evaluate hierarchical structures in stress-constrained design.

ENERGY STABLE RELAXATION-FREE RUNGE-KUTTA SCHEMES

Mohammad Reza Najafian Zadeh Najafabadi[*1] and Brian C. Vermeire*[1]

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ABSTRACT

Exact solution of the governing equations of physical phenomena often enforces auxiliary admissibility criteria, e.g., conservation of entropy or conservation of energies. Often referred to as invariants, these auxiliary admissibility criteria are typically not enforced via conventional discretization techniques. Ultimately, this leads to non-physical solutions, loss of accuracy, and loss of stability.

Over the past several decades, significant attention has been placed on low-order entropy or kinetic energy conservative spatial discretizations. These frameworks then have been extended to high-order discretizations, including discontinuous Galerkin (DG) and flux reconstruction (FR). For example see the work of Chan [1]. However, less attention has been given to the role of time integration on conserving invariants.

Recently, Ketcheson [2] demonstrated the relaxation Runge-Kutta (RRK) schemes can be used to enforce energy conservation, subsequently extended to entropy conservation by Ranocha et al. [3]. These introduce a time step relaxation parameter to enforce global conservation. In contrast, the incremental direction technique (IDT) can used to maintain a constant step size, but yields a loss of order of accuracy. Hence, existing techniques are disadvantageous, requiring dynamic variation of the step size, or loss of accuracy.

Here we introduce relaxation-free Runge-Kutta (RFRK) schemes, enforcing conservation while maintaining both a constant time step size and equivalent or greater order of accuracy than the base Runge-Kutta scheme. Implementation complexity is similar to that of RRK and IDT schemes and, under smooth solutions, performance converges to that of the base RK scheme. We demonstrate energy conservation for a range of example applications, and propose that these schemes are a suitable replacement for RRK and IDT schemes, alleviating the limitations of both previously proposed approaches.Exact solution of the governing equations of physical phenomena often enforces auxiliary admissibility criteria, e.g., conservation of entropy or conservation of energies. Often referred to as invariants, these auxiliary admissibility criteria are typically not enforced via conventional discretization techniques. Ultimately, this leads to non-physical solutions, loss of accuracy, and loss of stability.

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Relaxation Runge–Kutta Methods: Fully Discrete Explicit Entropy-Stable Schemes for the Compressible Euler and Navier–Stokes Equations. SIAM, 42(2):A612–A638, 2020.

Innovations in machine learning-enhanced uncertainty quantification for computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTI-FIDELITY MODELING FOR UNCERTAINTY QUANTIFICATION OF A RATCHETING MECHANISM

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ABSTRACT

Complex mechanisms containing gears, springs, and movable pawls are common in mechanical systems and are critical for the correct function of components that rely on subsystem kinematics to operate (e.g., mechanical watches). These systems involve contact interactions between various piece-parts during operation, which complicates their analysis because linearization of these systems is often infeasible. An approach to evaluate the performance of these mechanisms under relevant dynamic environments is to perform detailed, high-fidelity finite element analysis considering frictional contact. However, these types of simulations are very computationally intense and are often intractable when it comes to evaluating the performance of the structure over long periods of time, such as random vibration. Alternatively, simplified models and reduced-order models are efficient in terms of the computation times due to their lower-fidelity but may be limited in how accurate they are in terms of representing the physics. This work explores the use of a multi-fidelity machine learning surrogate model to combine multiple physics-based model fidelities to obtain a predictive model that achieves accuracy comparable to high-fidelity simulations with increased efficiency even when compared to a low-fidelity model. The proposed approach makes use of a Bayesian neural network to account for epistemic and random uncertainty, and the surrogate is used to study the mechanism’s response to varying inputs and parameters. The approach is demonstrated on a ratcheting gear mechanism that is relevant to industrial applications. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

CONSTRAINED PROBABILISTIC MODEL CALIBRATION GIVEN SUMMARY STATISTICS

Habib Najm[*1], Tiernan Casey[1], Pieterjan Robbe[1] and Mohammad Khalil[1]*

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ABSTRACT

Uncertainty quantification in computational models relies on probabilistic characterization of uncertain model inputs and parameters, which is effectually arrived at by the solution of a statistical inverse problem given available data. In this talk, we address specific challenges with the computational solution of statistical inverse problems in a Bayesian setting, related to missing data. In many practical situations, actual data is simply not available, and one is limited to available data summaries, in the form of statistics, such as nominal values and conditional/marginal bounds, on the quantities of interest or functions thereof. Maximum entropy methods are useful for inference employing constraints, rather than data. We describe our computational implementation of the maximum entropy principle employing approximate Bayesian computation methods, to enable inference of uncertain parameters given summary statistics that define a constraint on the data conditioned on all available information. We present illustrations of the performance of this construction in model application problems.

Microstructures of chemically complex materials and their impacts on material properties from multiscale simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MICROSTRUCTURE OF 2D RUDDLESDEN-POPPER PEROVSKITES USING LARGE-SCALE MONTE CARLO SIMULATIONS ENABLED BY MACHINE LEARNED POTENTIAL ENERGY MODEL

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ABSTRACT

2D layered lead-halide perovskite material has been the focus of intensive investigation in recent years due to its superior stability against the elements compared to the 3D counterparts, which is a consequence of intercalation of large organic hydrophobic spacer cations within its structure solving the degradation issue. Spacers induced quantum and dielectric confinement leads to different exciton binding, and hence, band gap values for different number of perovskite layers between the intercalating bulky organic molecules, thus enabling the tuning of the optoelectronic and photovoltaic properties in devices employing 2D perovskite material. To this day the theoretical studies of this material have been limited to density functional theory, and hence, several hundred atoms due to lack of reliable potentials which would enable the insight into the properties of the 2D perovskites observable in larger scale. In this study we developed quantum accurate machine learning enabled inter-atomic force-field based on the spectral neighbor analysis potential (SNAP) scheme applicable to most studied intercalating spacers butylammonium (BA) and phenylethylamonium (PEA). Our resulting SNAP potential reproduces the energies of the reference structures with high fidelity, while at the same time exhibits excellent stability in molecular dynamics simulations. We employed our machine learning enabled force-field to study layer distribution in 2D perovskite material including both of the aforementioned spacers by employing hybrid Monte Carlo approach. Our results from large scale Monte Carlo simulations are in good agreement with available experimental findings confirming non-uniform perovskite layer distribution between the intercalating cations. Furthermore, our results indicate that the non-uniform distribution is more energetically favorable compared to the uniform one which is a consequence of intricate balance between spacer and perovskite layer content which predominantly influences lead-halide bond properties. In addition, our simulations confirmed both temperature and spacer layer distribution dependence as predicted by the reference experimental study. Hence, presented multiscale simulations demonstrate that machine learning enabled models can be successfully employed to extract the microstructure of the complex perovskites and its impact on the underlying properties of the material.

Minisymposium in honor of Prof. Yannis Kallinderis's 60th birthday: Progress of Unstructured grid based CFD, hybrid mesh generation and adaptation, and parallel supercomputing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMMUNICATION-COMPUTATION OVERLAPPING FOR PARALLEL MULTIGRID METHODS

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ABSTRACT

Preconditioned iterative methods based on the Krylov subspace technique are widely employed in various scientific and technical computing. When utilizing large-scale parallel computing systems, the communication overhead tends to increase with the growth in the number of nodes, making its reduction a crucial challenge. In parallel finite element methods (FEM) and finite volume methods (FVM), halo communication and computation overlapping (CC-Overlapping) are commonly employed, often in conjunction with the dynamic loop scheduling feature of OpenMP. This approach has been primarily applied to sparse matrix-vector products (SpMV) and explicit solvers. Previous studies by the author have proposed reordering techniques for applying CC-Overlapping to processes involving global data dependencies, such as the Conjugate Gradient method preconditioned by Incomplete Cholesky Factorization (ICCG). Successful implementations on massively parallel supercomputers demonstrated high parallel performance, but the application of CC-Overlapping was limited to SpMV. In the present work, the author propose a method to apply CC-Overlapping to the forward and backward substitutions of the IC(0) smoother of the parallel Conjugate Gradient method preconditioned by Multigrid (MGCG). Using up to 4,096 nodes on Wisteria/BDEC-01 (Odyssey) with A64FX, performance improvements of approximately 40+% was achieved compared to the original implementation, while improvement was 20+% on Oakbridge-CX system with Intel Xeon CPU's.

Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RBF-BASED SURROGATE MODEL FOR COMPUTATIONAL HOMOGENIZATION OF ELASTOPLASTIC COMPOSITES FOR FINITE DEFORMATION

Akari Nakamura[*1], Yosuke Yamanaka[1], Shuji Moriguchi[1] and Kenjiro Terada[1]*

[1]*Tohoku University*

ABSTRACT

This study proposes a surrogate homogenization model of elastopolasic composites within the finite deformation framework using a Radial Basis Function (RBF) interpolation.
Although various homogenization methods have been developed so far, conventional methods, such as coupled and decoupled schemes, face challenges of high computational cost and complicated macroscopic constitutive model, respectively. In an attempt to overcome these problems, data-driven multiscale methods were developed by incorporating mechanistic machine learning technologies [1]. In this context, we have developed a data-driven method for two-scale analysis of elastoplastic composites under small deformation problem [2]. Specifically, the surrogate model was created by performing RBF interpolation for a constitutive database of macroscopic behavior of elastoplastic composite to replace the microscopic analysis in the two-scale analysis. However, it needs to be extended to the finite deformation framework to properly capture the multiscale mechanics of composite structures in practical problems. For that purpose, we changed the variable setting of the RBF interpolation from the infinitesimal strain and Cauchy stress to the macroscopic right stretch and the Second Piola-Kirchhoff stress. By employing these variables instead of the deformation gradient and First Piola-Kirchhoff stress, we can eliminate the influence of rigid body rotations in the proposed model. Also, we employ the right stretch tensor to define the history-dependent variables.

Representative numerical examples are presented to discuss the validity of the proposed method. As the first step, a series of numerical material tests are carried out on a representative volume element model composed of multiple elastoplastic materials to generate a constitutive dataset. To demonstrate the material flame-indifference of the presented method, we confirm the response of the model subjected to the large deformation involving rotation. Then, RBF interpolation is performed to the obtained dataset to create a surrogate homogenization model. Next, a macroscopic finite element analysis is conducted using the obtained model. Finally, localization analysis is performed using the macroscopic deformation gradient history at a certain computation point of the macroscopic structure.

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Numerical modeling of granular and multiphase flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A DEM-BASED SURROGATE MODEL FOR POWDER MIXING

Hideya Nakamura[*1], Naoki Kishida[1], Shuji Ohsaki[1] and Satoru Watano[1]*

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ABSTRACT

In many industries, powder mixing is an important operation. Numerical simulations based on the discrete element method (DEM) have been widely used for the analysis of the powder mixing process. However, high computational cost is one of the current limitations of DEM simulation. Recently, approaches combining machine learning models and numerical simulations have attracted considerable attention. However, high-speed computing methods that consider individual particle motions for powder mixing have not been investigated. Here, we present an original DEM-based surrogate model employing machine learning, namely, a recurrent neural network with stochastically computed random motion (RNNSR), which enables long-time scale powder mixing simulation with low computational cost and high accuracy. The RNNSR is designed to learn individual particle dynamics with periodicity from short-term DEM simulation results and predict powder mixing for a longer period of time. The RNNSR combines a recurrent neural network and a stochastic model to predict both convective and diffusive mixing. The simulation results obtained using the RNNSR were quite similar to those obtained using the DEM in terms of the degree of powder mixing, particle velocity, and granular temperature. It was also demonstrated that the RNNSR has the capability of ultrafast computation in powder mixing simulations. In conclusion, we have demonstrated the effectiveness of the RNNSR for ultrafast computation of the powder mixing process.

Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA ASSIMILATION-INTEGRATED MULTI-PHASE-FIELD SIMULATION OF SOLIDIFICATION IN SUS316L STAINLESS STEEL IN ADDITIVE MANUFACTURING

Shoichiro Nakamura[*1], Masahiro Kawasaki[1], Masahito Segawa[1] and Akinori Yamanaka[1]*

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ABSTRACT

Additive manufacturing (AM) is a powerful method to produce an industrial part with arbitrary shape and superior mechanical properties. In the AM process, extremely high cooling rates and thermal gradients cause formation of unique solidification microstructures. Since the unique solidification microstructures are formed very rapidly, it is challenging to observe their details experimentally[1]. Therefore, a numerical simulation is effective method to understand the mechanism of unique solidification microstructure formation in the AM process. The authors have recently developed the non-equilibrium multi-phase-field (NEMPF) model[2] coupled with the CALPHAD-based thermodynamic database to simulate the solidification behaviours in SUS316L stainless steel during the AM process. The NEMPF model describes the evolution of solidification microstructure and the partitioning of solute atoms at the solid-liquid interface in the non-equilibrium condition. However, the NEMPF model requires material parameters which are difficult to be identified and largely unknown. To solve the issue, Bayesian data assimilations (DA)[3] are effective because DA can estimate unknown material parameters and unobservable states through integration of simulation results and experimental data. In this study, we develop a new simulation methodology that couples the Bayesian DA with the NEMPF simulation of solidification in Fe-C-Cr-Mn-Mo-Ni alloys during the poder bed fusion (PBF) AM process. The numerical experiments called twin experiments are performed to validate the estimation accuracy of solidification state and material parameters obtained by the proposed method. The results of twin experiments show that the DA can accurately estimate the solidification state and material parameters (e.g., phase-field mobility) from only solidification microstructures. In order to obtain the accurate DA results, we reduce the computational cost of the NEMPF simulation by replacing the CALPHAD-based thermodynamic calculation with the machine learning method where the neural network estimates the Gibbs free energy and chemical potential from temperature and chemical composition at the solid-liquid interface region.

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Analytical models for nonlinear dynamics and evolved dynamics in natural, social and engineering sciences
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN INCREMENTAL TWO-STEP SOLUTION METHOD FOR SOLVING NONLINEAR DYNAMIC PROBLEMS

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ABSTRACT

The two-step solution was originally proposed for analyzing the cracking behaviors of concrete dams during strong earthquakes. 1) This paper reports an incremental two-step solution method for solving general types of nonlinear dynamic problems 2) A dynamic response problem in association with a time-dependent energy input is defined by four functions: the target function, T(x,y,z); the excitation function, E(t); the force function of T(x,y,z), FT(x,y,z,t); and the deformation function of T(x,y,z), DT(x,y,z,t). A nonlinear dynamic problem is expressed as $T(x,y,z) \times E(t) = FT(x,y,z,t)|NL \times DT(x,y,z,t)|NL$ (1)

The two-step approach suggests obtaining the force function FT (x,y,z,t)|L first by a linear response analysis, then an approximate nonlinear deformation function D*T(x,y,z,t)|NL is derived based on FT(x,y,z,t)|L by a static nonlinear analysis. This transforms the time history analysis from dynamic analysis to static analysis.

However, for a general type of nonlinear dynamic problem, the effect of nonlinearity in the deformation function DT(x,y,z,t)|NL on its dynamic response may be evaluated by the two-step solution at each time increment Δt during numerical computations, as

$T(x,y,z) \times E(ti + \Delta t) = FT(x,y,z,ti+\Delta t)|L \times DT(x,y,z,ti+\Delta t)|L$ (2)

$T(x,y,z) \times E(ti + \Delta t) \approx FT(x,y,z,ti+\Delta t)|L \times D^*T(x,y,z,ti+\Delta t)|NL$ (3)

Based on the solution of Eq.(2), the approximate nonlinear deformation function D*T(x,y,z,ti+Δt)|NL can be derived.

Note that the newly obtained incremental nonlinear features should be updated to the target function and the dynamic results should also be adjusted accordingly for subsequent analyses. This paper will show the effectiveness of this new method in solving dam crack problems.

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PSE (Problem Solving Environment)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT OF A MIXED REALITY VISUALIZATION SYSTEM USING A LOCATION-BASED METHOD FOR THE UNDERWATER OBJECTS

Ryodai Nakaso[1], Kazuo Kashiyama[1] and Tsuyoshi Kotoura[2]*

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[2]Penta-Ocean Construction Co.

ABSTRACT

Recently, the use of visualization based on MR (Mixed Reality) have been increasing in the several stage of construction work, such as planning, design, construction, maintenance and management. MR is effective in terms of safety because both hands are free and this feature is extremely effective in field use. We have developed a MR visualization system for the underground structures using marker-based method [1]. Although this method allows for highly accurate superimposition, it is necessary to set the marker at the correct position. On the other hand, the location-based methods using GNSS (Global Navigation Satellite System) receivers have been attracting attention in recent years. This method is particularly effective for visualization in open-sky environments or when there are no reference points around the objects, such as at the sea.

This paper presents the development of a MR visualization system using a location-based method for underwater objects. To obtain location information, GNSS receivers are used, which can obtain highly accurate location information by network RTK positioning at open-sky environment. The Microsoft HoloLens 2 is employed for the MR device. The system is capable of superimposed 3D models into real space accurately and automatically. The present system is applied to the visualization of underwater objects and flow simulation results in order to check the validity and effectiveness.

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New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTI-MATERIAL TOPOLOGY OPTIMIZATION USING MOVING WIDE SPLINE CURVES WITH CONSTRAINED ENDS

Hayate Nakayama[*1], Rixin Wang[2], Kozo Furuta[1], Benliang Zhu[3], Kazuhiro Izui[1] and Shinji Nishiwaki[1]*

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ABSTRACT

Topology optimization is a mathematical method that optimizes material distribution within a prescribed design space to maximize a desired performance while satisfying given constraints. For more practical applications, topology optimization methods that incorporate multiple materials have been developed. While solution frameworks based on density methods or level set methods that solve problems implicitly have been used for multi-material topology optimization conventionally, Zhang et al. established an approach for explicit multi-material topology optimization based on moving morphable components (MMC) method [1]. In MMC solution framework, a set of morphable components are used as building blocks to represent the structural topology explicitly. The optimal structure is obtained by optimizing the geometry parameters of these components such as widths, lengths, inclined angles, and locations. The advantage of this method is that the direct relationship between optimized structures and computer aided design (CAD) systems can be formed unlike the implicit way. However, in the MMC based method, there is an issue that fixed and input boundaries in the design domain are not connected by solid materials during the optimization process, which has a negative effect on its stability. To solve the disconnection issue, Zhu et al. proposed a single-material MMC based method that use moving wide Bezier components with constrained ends [2]. In this method, control points and widths of the Bezier curves are optimized, and their ends are constrained based on the boundary conditions.

Here, we propose a multi-material explicit topology optimization using moving wide spline curves with constrained ends. The key concept of this method is M kinds of level set functions are constructed explicitly by using a set of wide spline curves. These level set functions are used to represent M material domains and void domain without overlap. To maintain connectivity during optimization, the ends of certain wide spline curves are constrained according to prescribed boundary conditions. In addition, minimum length scale control can be easily achieved without imposing additional constraints by setting the lower bound of widths of spline curves. We show our proposed method’s validity via numerical examples from several optimization problems.

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PSE (Problem Solving Environment)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ANTHROPOPHOBIC TENDENCY AND SUBJECTIVE WELL-BEING

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ABSTRACT

Research suggests that Anthropophobic Tendency tends to increase over time. Another research revealed a negative correlation between well-being and perceived stress. And stress studies have shown that interpersonal relationships are stressors for the mental health of children and students. These findings suggest that the impact of interpersonal stress is an important issue in educational situations. We hypothesised that coping with stress would improve mental health and well-being. Therefore, the hypothesis of this study was that good coping with interpersonal stress would reduce anthropophobic tendency. The scales used were the Anthropophobic Tendency Scale (ATS), the Subjective Well-Being Scale (SWBS), and the Interpersonal Stress-Coping Inventory (ISI)'. ATS to see what kind of worries interpersonal phobia you have, SWBS to see what kind of cognitive and emotional aspects of subjective well-being you have, ISI to see what kind of positive attitude you have towards the stressful event, self-reflection and positive relationship coping. This involves taking positive actions to establish, improve and maintain positive relationships, including taking care of the other person who caused the stress, not getting involved with the other person, not talking to them, etc., and negative relationship coping, which is coping in which the person actively abandons or does not talk to the other person. Positive relationship coping, which is coping in which the person acts to establish, improve and maintain positive relationships, including being considerate of the other person, and negative relationship coping, which is coping in which the person actively abandons or disrupts the relationship, including not engaging with and not talking to the other person. The selection was made to see which of the following types of coping were more common. Postponing resolution coping is where the stressful events caused by the relationship are downplayed and avoided as a problem, such as not caring or thinking they can manage the problem by themselves. The results of an analysis of covariance using the data from those responses showed that positive relational coping had a positive effect on subjective well-being, and that subjective well-being had a negative effect on the anthropophobic tendency of the group. In this study, the relationship between subjective well-being, interpersonal stress coping and anthropophobic tendency was examined and it was found that learning positive relational coping in an educational setting and increases well-being and reduces anthropophobic tendency.

EFFICIENT DERIVATIVE-FREE OPTIMIZATION OF STRUCTURES OPERATING IN COUPLED FLUID-SOLID ENVIRONMENTS

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ABSTRACT

The bottleneck for optimizing mechanical structures operating in a fluid-solid coupled environment is often the fluid subsystem, due partly to the extensive degrees of freedom required to delineate the system. The objective however is to define the structure's geometry, material, or topology to maximize performance based on specified constraints. Coupling between fluid and solid subsystems relies on communicating the state variables at the domain intersection. Hence, substituting a surrogate fluid model that preserves the crucial flow feature – such as the interaction of shock waves with the structure – like, linear regression, Reduced Order Method, Neural Networks, etc., for a full-order fluid dynamics model to predict the interface state variables would provide a significant speed-up. This surrogate model could be trained in an offline-online framework where the database is created by sampling the design space uniformly, randomly, or in a greedy manner. However, this adds an expensive overhead to the optimization process.

We leverage these facts along with the data-based nature of derivative-free methods like Genetic Algorithm, Particle-Swarm, etc., to train an adaptive machine learning model on the fly and reduce computational costs. The database is dynamically created during optimization by storing the state variables such as pressure and displacement, at the material interface in a tree-type data structure and labeling these as ground truth. A simple mesh-free radial basis interpolation approach is adopted to predict the interface pressure showcasing the effectiveness of the proposed framework. During design iterations, an active learning-based classification model adaptively identifies new design points that can be evaluated using interpolated fluid pressure instead of pressure computed by the fluid dynamics solver. This model is chosen as it offers accurate predictions using limited training instances through interactive queries in regions of uncertainty. The proposed framework is versatile and applicable to any coupled problem involving an interface boundary condition.

To demonstrate this nested analysis and design framework, we investigate the weight reduction of blast mitigation chambers through geometry and wall-thickness optimization. The shock-dominated multi-phase FSI problem is simulated using the open-source finite element solver, AERO-S, and finite volume solver, M2C. Details of simulating strong shocks and their interaction with lightweight chambers capable of undergoing large plastic deformations will be discussed, along with optimization results.

Multiphysics and data-driven modeling for cardiovascular biomedicine
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A COMPREHENSIVE BENCHMARK FOR MYOCARDIAL MECHANICS

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ABSTRACT

Introduction
As cardiac biomechanical models are reaching maturity, and in anticipation of their wide use bedside, novel computational methods are being developed to increase model fidelity or computational efficiency. This process requires the validation of these methods and the comparison of their accuracy to established techniques. However, the lack of a real “ground truth” presents a problem and colleagues often revert to, either employing oversimplistic analytical paradigms, or, to computational phantoms where the effects of the computational methods choices employed in the phantom and the inherent numerical errors, may confound results. To address these needs, in this contribution, we present a series of analytically derived data sets for benchmarking myocardial mechanics and motion tracking.

Materials and Methods
We generated in silico datasets based on two axisymmetric geometries, traditionally used to model cardiac mechanics: a thick walled cylinder and a thick walled sphere. These reference geometries are subjected to a series of volume preserving, homogeneous deformations: (i). passive inflation, (ii). stretch and (iii). torsion, assuming quasistatic conditions. Adopting an incompressible, hyperelastic material description, we provide solutions for popular material models used in cardiac mechanics. The analytical solutions are implemented in MATLAB R2021b (MathWorks, Natick, MA, USA).

Results
We developed a benchmarking data set that can accommodate different needs raised by the community. The user is requested to select the reference geometry of the data set, the material description and deformation, and our code provides the continuous kinematics & dynamics, the corresponding boundary conditions, as well as estimates of work and energy. An additional functionality can provide meshes of the reference and deformed geometries with user specified resolution and interpolation schemes. Alternatively user specified meshes can be used as input.

Discussion and Conclusions
Through this work we make publicly available a benchmark for cardiac biomechanics based on analytical solutions of baseline problems in nonlinear mechanics. The resulting data set allows the user to test their methods against benchmarks of increasing geometrical and deformational complexity, which should aid them to locate the problematic areas in their code in a systematic manner. This data set, despite its simplicity, represents the primary modes of deformation in myocardial mechanics (inflation, torsion) – a significant improvement from previously used analytical benchmarks used in the community.

Theory and application of provably-robust and efficient high-order methods for high-fidelity computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PROVABLY-STABLE PARTITIONED ALGORITHM FOR CHT PROBLEMS

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ABSTRACT

In this work, we design and analyze a novel provably-stable partitioned algorithm for the conjugate heat transfer (CHT) problem. In the monolithic approach, a single numerical solver is developed to solve for all unknowns simultaneously. In contrast, a partitioned approach applies two separate solvers in each of the sub-domains, which are sequentially solved. Monolithic solvers are computationally efficient and robust but need to be designed for each new multi-physics problem, while partitioned schemes can take advantage of existing solvers. On the other hand, many partitioned schemes may encounter stability issues. As a model, we consider a CHT problem consisting of linear advection–diffusion and heat equations coupled at an interface and design a partitioned SBP-SAT scheme in each subdomain. In the proposed approach, the separate SBP-SAT schemes for each sub-problem are explicitly and weakly coupled at the interface. We proved that the resulting fully discrete scheme is conditionally stable dependent on specific range of SAT parameters.

WORKING TOWARDS A MODULAR, FULLY-COUPLED PHASE FIELD FRACTURE MODEL INTEGRATING ELASTICITY, PLASTICITY, AND DAMAGE

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ABSTRACT

Many phase field fracture models that have been implemented to date are opinionated regarding the choice of elastic model, plastic model, damage model, etc. While this enables easier development of the formulation itself, the resulting model is inflexible and often only applies to a subset of problems of interest. Further, if a change in model is desired, it may be required to redo much of the derivation and implementation. This work aims to develop and implement a generalized, variational, fully-coupled, and modular phase field fracture formulation capable of handling a diverse range of problems. The choices of elastic model, plastic model, damage model, rate-(in)dependence, degradation functions, and tension-compression split are all modularized with well-developed interfaces, enabling the development of solver infrastructure independent from the particular choices of models. While this approach brings its own challenges, it also enables classes of models which were previously tedious to implement, thus allowing the exploration of more complex problems.

In this presentation, we detail this modular approach from analytical derivations through to implementation in SIERRA, a robust multi-physical finite element code developed at Sandia National Laboratories. The approach will be demonstrated for several canonical model forms, including elastic and elastic-plastic fracture mechanics.

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High order methods for time-dependent problems
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HIGH-ORDER IMPLICIT SHOCK TRACKING FOR TIME-DEPENDENT FLOWS

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ABSTRACT

Shock tracking aims to generate a mesh such that element faces align with shock surfaces and other non-smooth features to perfectly represent them with the inter- element jumps in the solution basis, e.g., in the context of a finite volume or discontinuous Galerkin (DG) discretization. These methods lead to high-order approximations of high-speed flows and do not require nonlinear stabilization or exten- sive refinement in non-smooth regions because, once the non-smooth features are tracked by the mesh, the high-order solution basis approximates the remaining smooth features. High-Order Implicit Shock Tracking (HOIST) recasts the geometrically complex problem of generating a mesh that conforms to all discontinuity surfaces as a PDE-constrained optimization problem. The optimization problem seeks to determine the flow solution and nodal coordinates of the mesh that simultaneously minimize an error-based indicator function and satisfy the discrete flow equations. A DG discretization of the governing equations is used as the PDE constraint to equip the discretization with desirable properties: conser-vation, stability, and high-order accuracy. By using high-order elements, curved meshes are obtained that track curved shock surfaces to high-order accuracy. The optimization problem is solved using a sequential quadratic programming method that simultaneously converges the mesh and DG solution, which is critical to avoid nonlinear stability issues that would come from computing a DG solution on an unconverged (non-aligned) mesh [1] .
In this work, the HOIST method is further extended to simulate time-dependent, inviscid flows for higher dimensions. We use a space-time formulation of the governing equations and perform shock tracking over a space-time slab [2]. In the two-dimensional space and time setting we generate a three- dimensional mesh by extruding a spatial mesh of quadrilateral elements into hexahedral elements. We also introduce robustness measures for hexahedral element collapses, as well as a method to leverage information from previous time-slabs to improve the initial guess for our mesh on the current slab.

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Advanced discretization schemes and solution strategies for computational structural dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MATRIX ANALYSIS OF MOLECULAR STRUCTURES: FORMULATION AND STRATEGIES FOR SOLVING THE COMPUTATIONAL DYNAMICS PROBLEM

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ABSTRACT

Although viruses may seem to be infinitesimal biological entities, harmless for the future of the human species, SARS-CoV2 has put the whole of humanity in check, causing millions of deaths. In such a situation, it is worth considering the possibility of developing new methods for disabling or deactivating the viral structures.

In the field of structural engineering, vibration frequencies are determined so that structures such as bridges do not collapse. But the opposite approach could also be considered, i.e.: calculating the vibration frequency for which a structure such as a virus could collapse by resonance. If the natural vibration frequencies of a molecular structure were known, a device could be constructed that would cause the virus enter into resonance until its collapse, as if it were the old Tacoma Narrows bridge.

In the framework of the VirionBreak project, developed by the GMNI with funding from the Instituto de Salud Carlos III (ISCIII), a formulation was proposed that allows the definition of the mass and stiffness matrices in a structure with intramolecular bonds, which is the first step in the calculation of the vibration frequencies of the structure [1]. The proposed formulation allows the analysis of any three-dimensional structure with the characteristic bonds that are considered in the molecular dynamics field, i.e., stretch, angular and dihedral type bonds, including their possible degenerate configurations [2].

The formulation has been applied to a series of molecules, comparing the results obtained with theoretical and experimental values from different sources, obtaining a good fit in all the cases analyzed [3]. The formulation can also be applied to the calculation of vibrational frequencies of arbitrarily large complex structures, such as viruses, where the intramolecular bonds considered are the causes of structural integrity.

The strategies for solving these particular type of computational dynamics problems are discussed.

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Immersed-boundary variational methods: Theory, data structures, and applications
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STABILIZATION STRATEGIES FOR THE 3D CARTESIAN GRID DISCONTINUOUS GALERKIN METHOD (CGDG)

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ABSTRACT

Simulating the propagation of waves through a complex domain involves significant computational challenges. High order finite element methods have proven to be one of the best simulation alternatives, capable of providing accurate and efficient solutions. However, robust techniques for automatically generating the curved meshes required for these analyses still remain challenging.

The Cartesian grid discontinuous Galerkin finite element method (cgDG) [1] represents an advancement in this regard. The method's main features include the use of high order discretizations within Cartesian meshes independent of the geometry, together with the formulation of the weak form of the problem following the discontinuous Galerkin (DG) approach. As a result, the meshing process becomes trivial, computation times can be significantly reduced, and the solution approximation retains the properties of conventional high-degree methods. The strategy was introduced for the 2D case in [1] and applied with great success to solving problems related to electromagnetic scattering.

This work presents the extension of cgDG to the 3D context. Generalizing the method requires refining the strategies developed for the 2D case, such as element overlap and domain reassignment. The method is implemented to solve the Maxwell equations in the temporal domain, and its performance is evaluated in a series of reference problems.

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Biomechanics of hard tissues: From experiments and simulations to clinical applications
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COMPUTATIONAL STUDIES ON THE POSSIBILITY OF MG IMPLANTS FOR HARD-TISSUE APPLICATIONS

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ABSTRACT

The choice of implant material at the fracture site has an influence on the fracture healing not only from the biological perspective but also from the mechanical perspective. Biodegradable implants such as magnesium (Mg) and zinc (Zn) have shown to fasten the secondary bone healing process as compared to that of bioinert implants such as titanium (Ti). In general, this benefit of Mg was seen mostly only from biocompatibility perspectives. However, the advantage of Mg is also there in terms of mechanical perspectives.

We studied the effect of Ti and Mg as base materials for implants from mechanical perspectives in the initial phase of bone healing. The focus was on the displacements at the fracture site of the tibia and their influence on the stimulus for bone healing. Claes tissue differentiation theory was used to evaluate the conditions for secondary healing at the callus. In addition, the stress distribution in the implant determined in order to quantify the change in the stress shielding conditions. In comparison, Mg implants have minimal stress shielding problem than Ti, which led to better mechanical stimulus at the fracture site. The conditions for secondary bone healing were better when Mg implants were used. The study illustrates the benefits of Mg for osteological implants from mechanical perspectives and the potential to replace Ti for fracture treatment in the future.

Constitutive modeling of complex materials with machine learning and artificial intelligence
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DIFFERENTIABLE FEM FOR NEURAL CONSTITUTIVE MODELING OF COMPLEX MATERIALS

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ABSTRACT

Understanding and predicting the constitutive behavior of materials with complex microstructures pose significant challenges in materials science, primarily due to the resultant nonlinear macroscopic properties, which are further complicated by mechanisms like viscoelasticity, plasticity, and damage at the sub-scale level. Traditional constitutive models, evolving since their inception in the early 19th century, have gradually incorporated complex physics but often fail to address the intricate interplay of microstructural behaviors effectively. The application of machine learning, specifically neural networks, for constitutive modeling has emerged as a promising avenue in the past decade. These approaches offer a paradigm shift from conventional physics-based and phenomenological models, providing a novel perspective for learning complex material behavior from data. However, existing neural network-based models are critically dependent on the availability of extensive, high-quality datasets of direct measurements, largely limiting their practical applicability. Furthermore, the integration of neural networks with traditional numerical solver, especially for indirect data management, presents the technical challenge of propagating essential intermediate gradients for a holistic optimization. Physics-informed learning approaches, e.g., PINN, while addressing some of these limitations, are constrained by their training and convergence challenges in many complex scenarios. In response to these challenges, this study introduced a novel neural differentiable modeling framework that seamlessly integrating deep neural network with differentiable FEM solver to effectively learn and discover the constitutive laws of complex materials from indirect data, offering a robust and scalable solution to the longstanding challenges of modeling complex material behaviors.

A QUALITY BY DIGITAL DESIGN (QBD2) FRAMEWORK FOR THE DEVELOPMENT OF INTENSIFIED CRYSTALLIZATION SYSTEMS

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ABSTRACT

Crystallization is an important unit operation in solid products manufacturing as it acts as not only a purification step but also a process control step for influencing crystals critical quality attributes (CQAs) such as crystal size, shape, and polymorphic form1. Efficient crystallization is prioritized for intensified manufacturing processes with high impact in the manufacturing of solid products for various industries, including energetic, pharmaceutical, food and fine chemicals. The integration of digital twins and digital design frameworks enhances and streamlines this process by providing a virtual representation of the crystallization process, allowing for detailed simulation and optimization across the design space. Resveratrol, a dietary supplement chosen as a model material for energetic substances, shares a similar chemical makeup to some traditional energetic materials and offers a safer alternative. A modular autonomous crystallization system (MACS) with a model-free Quality-by-Control (mfQbC) approach minimizes required experiments while utilizing feedback control to enhance the understanding of the system2. An automated design of experiments (DoE) through an in-house LabVIEW platform called Omnibus streamlines data collection. This DoE involved 6 heating-holding-cooling experiments with various cooling rates and seeding amounts to gain insights on crystallization mechanisms, such as primary nucleation, secondary nucleation, the metastable zone width tendencies, and nucleation rate. Direct nucleation control (DNC) and supersaturation control (SSC) experiments were applied to further improve the understanding of attainable regions and design space for the system and to generate data for model identication.1 Process analytical technology (PAT) tools collect in-situ data that can be translated into crystal size, concentration, and polymorphic form. Based on this information a process model was developed to include the mechanisms occurring, allowing for parameter estimation to then develop a digital twin using two-dimensional population balance modeling (PBM). This digital twin facilitates in silico investigation of the design space as well as the digital design of the crystallization process to achieve the desired CQAs. The results illustrate a systematic quality-by-digital-design (QbD2) framework for the understanding and development of optimized crystallization processes.

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PRATT TRUSS CHARACTERISTICS FOR OPTIMAL WEIGHT

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ABSTRACT

In recent years, two main trends can be observed in the research on topology optimizations. One is focused on optimization results, intended for additive manufacturing, while the other is oriented towards traditional construction production. Optimizations fitted for additive manufacturing holds great potential for the future and is approved topic among researchers. Optimization solutions contributing to traditional construction production, can provide immediate benefits for the industry. Pratt truss can be considered as specific subset from the ground structure domain. There can be found more efficient truss topologies than Pratt truss, but it is widely used and suitable for traditional production.

This study focuses on finding correlation between various Pratt truss characteristics and the truss weight. Aim is to define truss geometry based on certain parameters, that would give its weight close to optimal or optimal. Several parameters are set to analyze truss behavior within established model. Some of the characteristics are based on geometry, others are based on the principles of Force Density Method. Correlation is explored by using the advantages of parametric design and machine learning. The resulting data are obtained by calculating significant number of trusses using parametric model and Finite Element Method. Steel trusses with span $L \in \{12\ m \leq x \leq 25\ m\}$ and height $H \in \{1\ m \leq y \leq 3.55\ m\}$ are studied. For each truss case constant roof load is applied and two types of supports selected. To explore member profile impact on characteristics, they were defined as continuous and discrete variables. The obtained data are processed and analyzed using machine learning algorithms and by visually observing generated graphs and animated calculation process.

Data analysis revealed non-linear correlations between the selected parameters and truss weight. Approach for the profile choice affects correlation and the possibility of predicting the weight of the truss. Better understanding of the truss topology can reduce the time needed to obtain optimal solutions. Dataset displayed some outcomes that did not fit within the rest, revealing different behavior of the specific trusses compared to other. These distinct cases are planned to be studied in more detail in the future research.

Recent advances in numerical methods for mixed-dimensional PDEs
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELLING COUPLED SURFACE-BULK VISCOUS FLOWS IN ANIMAL CELLS WITH UNFITTED FINITE ELEMENTS

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ABSTRACT

The shape of animal cells is governed by the surface mechanics of its actomyosin cortex: a network of cross-linked polymer filaments stirred by active motors and lying beneath the plasma membrane [1]. In large animal cells, cortical actomyosin flows can drag cytoplasmic flows in the cell bulk, and vice versa [2]. These surface-bulk hydrodynamic couplings serve a myriad of biological functions, such as contributing to the establishment of PAR-polarity in the C. Elegans zygote, the even distribution of syncytial nuclei in Drosophila embryos or the asymmetric positioning of the spindle in mouse oocytes. However, they have been so far little investigated, due to a lack of appropriate numerical tools.

In this talk, we will describe our efforts to shed light onto this matter with mathematical modelling and numerical simulations with unfitted Finite Element (FE) methods [3]. Together with biophysical measurements, they can test current hypotheses, formulated by biologists and physicists, on the mechanisms ruling interactions between the cortex and the cytoplasm. The mathematical model considers the dynamics of surface-bulk viscous flows on general and smooth closed surfaces with an active term on the surface, representing active tensions generated by the activity of myosin motors. For the numerical discretization, we have considered a first-of-its-kind approach, coupling trace FE formulations for the surface physics with aggregated FE formulations for the bulk physics. We will provide details on our coupled formulation and its numerical behaviour, performance aspects of the computer implementation, and some numerical examples, including qualitative experimental validation.

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Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION FOR FIBER ORIENTATION IN FRACTURED CONCRETE

Andre Luis Ferreira da Silva[1], Luís A. G. Bitencourt Jr.[1] and Emilio Carlos Nelli Silva[1]*

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ABSTRACT

Concrete is widely used in civil engineering due to its compression strength. However, it is prone to cracking under tension, necessitating reinforcements to mitigate this vulnerability. The addition of fibers in the concrete has been used to improve the concrete resistance under tension solicitation after cracking occurrence. However, the orientation of these fibers plays a crucial role in the structure's mechanical behavior, making it possible to reduce the amount of fibers used to reinforce the concrete. The optimized fiber orientations are addressed in this work using the Topology Optimization.

The concrete behavior is simulated using a Continuum Damage Mechanics Theory (CDMT)-based model with a rate-independent formulation, distinguishing between tensile and compressive responses.

The methodology integrates an implicit-explicit integration scheme to improve computational efficiency. By focusing on the fracture mechanics model, we seek to minimize structure compliance, indirectly extending the lifespan of the reinforced concrete. We present the methodology, results, and conclusions, highlighting contributions to the field of concrete reinforced with fibers.

Computational methods in environmental fluid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INCORPORATION AND EVALUATION OF PARAMETRIC WIND AND RAINFALL MODELS FOR COMPOUND FLOODING IN A DISCONTINUOUS GALERKIN STORM SURGE FRAMEWORK

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ABSTRACT

Accurate meteorological data, encompassing wind, pressure, and rainfall, are crucial inputs to hurricane-related storm surge forecasts and hindcasts. These meteorological fields can be generated using simple parametric storm models, which are functions of a small number of key storm parameters like storm track, maximum winds, and radius of maximum winds. While the National Hurricane Center's advisory (for forecasts) and best-track (for hindcasts) data are routinely used to inform parametric wind and pressure fields in storm surge models, the inclusion of rainfall is typically omitted, resulting in an incomplete flood assessment during hurricanes, which are often accompanied by extreme precipitation. We aim to address these gaps in storm surge modeling through incorporation of a parametric rainfall model (known as R-CLIPER), enabling accurate and efficient modeling of the meteorological drivers of compound flooding events. In this talk, I will discuss our efforts to improve simulations of compound flooding events due to both surge and rainfall through incorporation of the parametric rainfall model into a discontinuous Galerkin shallow water equation model (DG-SWEM). Evaluations of multiple enhanced storm surge simulations for hurricanes with varying intensities of accompanying rainfall will be presented.

A MULTI-QUERY MODEL REDUCTION FRAMEWORK FOR NONLINEAR DYNAMICS SIMULATIONS WITH MULTIPLE NON-PARAMETRISED LOADING CONFIGURATIONS

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ABSTRACT

Predicting the service life and assessing hazards for a complex structure under various loadings poses a recurrent challenge, particularly pronounced when evaluating the risk of structural failure due to seismic hazards, which often entails numerous computationally intensive simulations. For example, when constructing fragility curves, the nonlinear damageable behavior of structures needs careful consideration, necessitating dynamic response computations for a broad spectrum of potential ground motion inputs.

In such scenarios, model reduction techniques emerge as powerful strategies, leveraging computational similarity to expedite the sequence of calculations. The LATIN-PGD method proves instrumental in efficiently handling the nonlinear aspects of the problem. Simultaneously, the efficient management of parametric problems is achieved by constructing a reduced-order basis applicable across all scenarios.

This research extends the application of the LATIN-PGD method to dynamic problems and introduces an innovative approach for efficiently addressing cases where loadings cannot be easily parameterized. To address this, a space-frequency PGD is introduced for solving the dynamics aspect of the history-dependent nonlinear problem, thereby combining the effectiveness of model-order reduction with the numerical advantages of frequency computations. Additionally, a novel approach is introduced to handle multi-query aspects, enabling a highly efficient linkage of computations. The resulting computational cost is significantly reduced compared to the cumulative expense of independently executing various scenarios.

CONSERVATION PROPERTIES OF EMBEDDED FINITE-ELEMENT METHODS FOR FLOW IN FRACTURED POROUS MEDIA

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ABSTRACT

Numerical simulations of Darcy flow in fractured porous media rely on hybrid- or equidimensional fracture models. The former considers fractures as lower-dimensional manifolds, while the latter treats them as objects of the same geometrical dimension as the porous matrix. Embedded strategies are widely used simulation approaches that remove the inherent difficulties in mesh generation for fractured media, as they employ two different and possibly non-conforming meshes.

Among all possible embedded approaches, we focus on strategies that rely on the Lagrange multiplier method and are discretized within a Continuous Galerkin (CG) finite-element framework [1]. From a theoretical perspective, we analyze the conservation properties [2] of embedded discretizations based on non-conforming meshes. Following that, we present a computational analysis for both hybrid and equidimensional models of fractures, considering established benchmarks for flow in porous fractured media.

The numerical results confirm that embedded discretizations are conservative on subdomains consisting of unions of elements.

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Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

URBAN MULTI-PHYSICS CFD MODEL TO ACCESS THE COOLING POTENTIAL OF TREES IN A TYPICAL NORTH AMERICA NEIGHBORHOOD

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ABSTRACT

In a world strongly affected by climate change, understanding complex urban climate phenomena by explicit Computational Fluid Dynamics (CFD) modeling stands out as a crucial pursuit. Since cities are heating up, research studies need to address appropriate heat-mitigation solutions to enhance thermal comfort relying on comprehensive analysis of urban environment. Among other mitigation measures, trees can reduce the ambient heat by providing shading and transpirative cooling. However, trees also come with potential negative effects such as ventilation reduction by impeding incoming wind, the increase of relative humidity due to the moisture release by leaves, or the sky view factor reduction, ultimately reducing thermal comfort.

This complexity warrants CFD studies to understand the cross-effects of trees towards an optimal balance. This study assesses the overall contribution of urban trees on pedestrian comfort according to different vegetation scenarios. To explore the urban complexity, the study uses a homemade CFD-based coupled solver developed by authors called urbanMicroclimateFoam, based on OpenFOAM. This urban microclimate model solves successively fluid motion with realizable k-ε RANS, heat and moisture (HAM) transport in porous media, and radiative exchanges including multiple diffuse reflections, in three distinct sub-domains with their respective meshes. Regarding temporal coupling, for each steady RANS time step performed, transient HAM simulations are conducted with adaptive timesteps using Picard iterative scheme.

Downscaling from results obtained through mesoscale meteorological model WRF, time-varying boundaries conditions are established. To reduce gravity wave reflection, blending layers are imposed on lateral boundaries where velocity and temperature are relaxed.

The study relies on a model of a typical neighborhood in Montreal representing six lots for a total study zone of 250m x 300m. One major challenge is managing a wide urban model with different sub-meshes while maintaining acceptable precision and computational cost.

Universal Thermal Climate Index (UTCI) combining air temperature, mean radiant temperature, velocity and relative humidity at a given position documents outdoor thermal comfort. Analysis demonstrates that trees in ventilation corridors, aligned with the primary wind, reduce the mean pedestrian comfort by wind blocking despite the shade generated. On the other hand, trees in private gardens, or in crosswind corridors, can enhance both the local thermal comfort and the overall mean pedestrian comfort over the entire neighborhood, thereby improving overall walkability. As a final aim and based on those findings, the

present study will propose an ideal vegetation configuration maximizing cooling potential and pedestrian comfort.

Modeling and simulation of coupled processes in geological media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TRANSPORT OF MICROCAPSULE IN FRACTURED MEDIA USING COUPLED CFD-DEM METHODS

Pania Newell[*1] and Xiaoming Zhang*[1]

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ABSTRACT

Geothermal energy presents a promising solution to address our energy crises and environmental concerns. However, challenges such as production temperature, flow rate, and thermal breakthrough time impact its efficiency. In this presentation, we propose an innovative solution involving the injection of polymer-based microcapsules into fractures to modify permeability and prevent preferential flow, ultimately mitigating thermal breakthrough. Utilizing coupled computational fluid dynamics and discrete element method (CFD-DEM), we investigated scenarios considering microcapsule size, concentration, and fracture roughness. Our findings reveal that in smooth fractures, small microcapsules easily traverse, while larger ones do so at lower concentrations, and a mixture of sizes tends to seal the fracture. In rough fractures, microcapsule transport complexity increases due to interactions with rough walls. The results suggest that complex fracture surfaces enhance sealing behavior, and this effect could be alleviated using smaller and lower concentrations of microcapsules.

Recent advances in high-order methods for computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DISCONTINUOUS GALERKIN METHODS FOR HYPERSONIC FLOWS

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ABSTRACT

In recent years, high-order discontinuous Galerkin (DG) methods have emerged as an attractive approach for numerical simulations of compressible flows. We present an overview of the recent development of DG methods for compressible flows with particular focus on hypersononic flows. We describe various shock capturing methods to deal with strong shock waves in hypersonic flows. We discuss r-adaptivity techniques to refine meshes for hypersonic boundary layers. We present a few examples to demonstrate the ability of high-order DG methods to provide accurate solutions of hypersonic laminar flows. Furthermore, we present direct numerical simulations of hypersonic transitional flow past a flared cone at Reynolds number 10.8×10^6, and hypersonic transitional shock wave boundary layer interaction flow over a flat plate at Reynolds number 3.97×10^6. These simulations run entirely on hundreds of graphics processing units (GPUs) and demonstrate the ability of DG methods to directly resolve hypersonic transitional flows, even at high Reynolds numbers, without relying on transition or turbulence models.

Multi-scale, multi-rate damage and fracture: Models, experiments, and simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE ROLE OF SURFACE DEFECTS IN DYNAMIC DUCTILE FAILURE: AN EXPERIMENT AND NUMERICAL STUDY

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ABSTRACT

In this work, we study the role of surface defects on ductile damage evolution during dynamic loading process on polycrystalline copper. The surface defects of different shapes and locations were manufactured on the surface of the target specimens subjected to impact experiment. The velocity history of each experiment was recorded for diagnostic purposes. In addition, the target specimens were sectioned after the experiments for microstructure analysis. The resulting velocity signals and the microstructures (of the loaded specimen) shows a strong effect of the defect shape and location. The experiments were modeled with a calibrated set of a viscoplasticity model of Preston-Tonks-Wallace (PTW) and ductile damage model (Tepla). The simulations successfully capture the trend of surface defect dependence on both the velocity signal and the resulting microstructure. Examination of the evolving stress field within the target material under loading reveals the mechanism behind this surface defect dependence.

Industrial applications of IGA
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ISOGEOMETRIC ANALYSIS AND THE DIGITAL TWIN

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ABSTRACT

The Digital Twin represents a new digital frontier in industry, theorized to improve quality, improve efficiency in the product lifecycle, and open up new avenues for revenue and customer satisfaction. Product Digital Twins represent a particular product or assembly which is identified as the single source of truth however the design process of today currently does not align with the vision of utilizing that single source of truth. In many approaches to analysis of design, derivatives of the product design are produced to understand the impact of environmental requirements. This approach, with disparate or disconnected geometric derivatives, does not create a path towards the realization of the vision of the Digital Twin. Isogeometric Analysis is in a unique position to allow a direct connection to the singular ‘source of truth’ during the analysis process. It can be shown that IGA satisfies the Digital Twin’s direct connection to CAD or representative physical geometry. In addition, IGA has shown promise as the solution method for future designs that would include complex geometries produced by optimization methods and generative design. Also, a discussion on other technologies that are required to further enable the vision of the Digital Twin as it relates to mechanical simulation.

Causal discovery and graphical causal models
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CAUSAL SPATIAL STENCIL LEARNING: CAUSAL DYNAMICS IN COMPLEX SPACE-TIME SYSTEMS

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ABSTRACT

Discovering causal relationships is one of the foremost endeavors in science. With an ever increasing need to address anthropogenic climate change, understanding the etiologies of our climate's systems is essential. However, climate datasets are typically extremely high-dimensional, consisting of hundreds of variables measured across thousands of grid locations, which poses extreme difficulties for existing causal discovery algorithms. To escape this high dimensional regime, prior applications of causal discovery algorithms in climate science typically perform extreme spatial dimension reduction; this spatial dimension reduction, however, impairs the interpretability of the discovered relationships, and is particularly problematic when studying transient phenomena with rapidly changing spatial structure, such as volcanic eruption plumes. To address these issues, we present Causal Spatiotemporal Stencil Learning (CaStLe), a novel algorithm for discovering local dynamics in spatiotemporal systems. By projecting individual grid cells to a relative coordinate structure, CaStLe leverages implicit spatial replicates to identify uniform local dynamics, thereby eliminating the high dimensionality and reducing the sample complexity of the causal discovery task. We demonstrate the advantages of CaStLe through a comprehensive simulation study and application to a large-scale Earth system model. CaStLe achieves state-of-the-art results for discovering causal spatiotemporal dynamics and enables characterization of a wider range of climate dynamics.

Fracture, damage and failure mechanics of cementitious materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

3D MULTI-PHYSICS SIMULATION OF HIGH TEMPERATURE INDUCED THERMO-HYGRAL FRACTURE OF CONCRETE

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ABSTRACT

When exposed to fire, concrete is liable to fracture and spalling owing to thermo-hygro-mechanical phenomena. It is challenging to gain a deep and systematic understanding of high temperature induced cracking in concrete due to the interplay of several physical phenomena, some of which are non-linear. In particular, spalling is widely considered to be highly dependent on the migration, evaporation and condensation of internal moisture content. Numerical modelling may be the only viable method for studying high temperature concrete fracture phenomena, as the real time observation of moisture propagation, evolution of vapour content and induced pore pressure, and mechanical strain in 3D are difficult or infeasible to obtain by experimentation.

The model presented in this study simulates thermal conduction, multi-phase moisture diffusion, and the induced mechanical deformation and fracture owing to thermal gradients and build-up of pore pressure. Studies in this area are usually limited to 1D or 2D problems, despite the fact that cracking is inherently a 3D phenomenon. PDS-FEM was used as the numerical method since it provides a numerically efficient treatment for simulating crack propagation in large 3D models. The model was validated against experimental data [1] by comparing with the measured pressure and temperature at varying depths, where good qualitative agreement was met.

Using the validated model, a full 3D simulation was conducted in order to explore and compare the simulated fracture pattern with available visual data [2]. As a result of the observed results, we speculate that a build-up of moisture inside the macro-cracks may be a key mechanism responsible for spalling. Therefore, we also introduce a mechanism by means of an additional boundary condition for the release of moisture into the opened cracks. This has laid the groundwork for estimation of the additional macroscale pressure exerted on the concrete skeleton inside the cracks themselves.

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Transport phenomena in micro/nanofluids
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MANIPULATION OF CONTACT ANGLE HYSTERESIS AT ELECTRIFIED IONIC LIQUID-SOLID INTERFACES

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ABSTRACT

Room-temperature ionic liquids (RTILs) are intriguing fluids that have drawn much attention in applications ranging from tribology and catalysis to energy storage. With strong electrostatic interaction between ions, their interfacial behaviors can be modulated by controlling energetics of the electrified interface. In this work, we report atomic-force-microscope measurements of contact angle hysteresis (CAH) of a circular contact line (CL) formed on a micron-sized fiber, which is coated with a thin layer of conductive film and intersects a RTIL-air interface. The measured CAH shows a distinct change by increasing the voltage U applied on the fiber surface. Molecular dynamics simulations were performed to illustrate variations of the solid-like layer in the RTIL adsorbed at the electrified interface. The integrated experiments and computations demonstrate a new mechanism to manipulate the CAH by rearrangement of interfacial layers of RTILs induced by the surface energetics.

Theory and application of provably-robust and efficient high-order methods for high-fidelity computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HIGH-ORDER FINITE DIFFERENCE METHOD FOR INCOMPRESSIBLE NAVIER-STOKES EQUATIONS IN COMPLEX GEOMETRY

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ABSTRACT

We solve the incompressible Navier-Stokes equations in complex geometry using a multi-block high-order finite difference scheme with summation-by-parts (SBP) properties. The work is a continuation of the work in [2], with the continuation of curvilinear multi-block geometries. Using the Projection method [1] for interface and wall boundary implementations the boundary conditions are imposed strongly, as separate from the usual weak imposition of the Simultaneous-Approximation-Terms (SAT) boundary method commonly seen in SBP schemes. Something shown in [2] to improve the detail of near boundary effects, such as vortices. Using SBP operators the well-posedness analysis of the discrete scheme can be directly related via the Energy method to the continuous well-posedness analysis, showing energy conservation of the system. Stability for the scheme is proven using the Energy method for the curvilinearly transformed equations and convergence of expected order is shown for the analytic Taylor-Green vortex problem on complex coupled multi-block geometries. Classical benchmark problems, such as cylinder in flow are also solved.

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A HIGH-ORDER FAMILY OF 4-D CONFORMING ELEMENTS

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ABSTRACT

Therre is considerable recent interest in the design of high-order discretizations of PDEs in 4D (space-time problems). In this joint work with David Williams, we present families of conforming high-order finite elements on certain non-simplicial domains, which arise naturally in 4-D meshes. The constructions - which are explicit - rely on techniques from the finite element exterior calculus.

Geomechanics of the cryosphere
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXAMINING SEA-ICE FORMATION WITHIN THE CANADIAN ARCTIC ARCHIPELAGO USING DEMSI

Svetoslav Nikolov[1], Kara Peterson[1], Adrian Turner[2] and Devin O'Conner[1]*

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ABSTRACT

High resolution (sub-kilometer - 1 km) models are required to accurately resolve sea-ice formation within the Canadian Arctic Archipelago (CAA) due to the large density of islands and tortuous channels which surround them. To build these high resolution models we rely on a unique PCA-based data fusion methodology that leverages both active (synthetic aperture radar, SAR) and passive (thermal-infrared, TIR) satellite sensor data to accurately initialize sea-ice simulations. This data fusion procedure is integrated into the Discrete Element Method for Sea-Ice (DEMSI) code, which is a Lagrangian particle method capable of naturally handling the non-linear/discontinuous sea-ice behavior during fracture. Using these SAR-TIR data infused DEMSI simulations we examine how sea-ice growth progresses in Queen Elizabeth islands during the fall months. A comparison with coarser 20 km arctic basin DEMSI models and raw SAR/TIR data is provided.

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DEVELOPING A NOVEL LAYERWISE THEORY TO ANALYZE NONLINEAR FREE VIBRATION OF THERMALLY POST-BUCKLED FG-GRC THIN-WALLED STRUTS

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ABSTRACT

The influence of local buckling on the performance of slender structural elements subjected to compressive loads has been a significant focus within the industry. Specifically, for thin-walled sections, local buckling leads to a marked decline in axial compressive stiffness, which in turn considerably diminishes their load-bearing capacity. One of the main objectives of this paper is to examine the possible enhancements in fundamental frequencies and post-local buckling responses of polymeric composite laminated thin-walled struts, such as channel sections, under thermal conditions, through the use of multi-layer graphene sheet reinforcements. Owing to the graphene volume percentages variations in each layer constituting the webs and flanges of thin-walled structures, a piecewise functionally graded distribution is observed through their thicknesses. To precisely and efficiently analyze the nonlinear compressive behavior of these structures, a novel layerwise theory based on the third-order shear deformation theory by incorporating von Karman geometrical nonlinearity has been introduced. Laminated plate theories, commonly employed for plate and shell analysis, can be broadly categorized into two types: the equivalent single layer (ESL) theory and the layerwise theory. In both cases, the 3D elasticity problem is simplified into a two-dimensional (2D) problem. However, it is important to note that the ESL theory has certain limitations, particularly in accurately predicting stress and strain distribution in thick composite laminates or in situations involving dissimilar material layers, such as FG-GRC, where thermomechanical properties vary throughout the laminate's thickness. This limitation arises due to the assumption of constant transverse shear stresses throughout the thickness direction. To address these challenges and provide an accurate estimation of the post-local-buckling response of FG-GRC laminated channel section struts, this paper employs the layerwise theory in conjunction with the TSDT. To verify the accuracy of the results obtained based on the LW-TSDT and to evaluate its computational efficiency, a three-dimensional (3D) finite element model is also developed using ABAQUS for comparative analysis. An extensive analysis of nonlinear stability is performed on functionally graded graphene-reinforced composite (FG-GRC) laminated thin-walled struts to determine the optimal material distribution that raises both the critical buckling temperature and the pre/post- buckled fundamental frequencies.

Fluid-structure interaction in interface and moving boundary problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

3D GENERATIVE AI BASED ON DEEPSDF INCORPORATING STRUCTURAL DYNAMICS

Koji Nishiguchi[1], Issei Toida[1], Naoya Chiba[2], Yuji Wada[3], Rio Yokota[3], Hiroya Hoshiba[1] and Junji Kato[1]*

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ABSTRACT

We propose a deep generative model for 3D shapes that incorporates structural mechanics parameters and a dataset of about 10,000 3D shapes created by topology optimization and Eulerian elastoplastic simulation using Cartesian mesh. Our model is based on DeepSDF, a decoder-type neural network that implicitly represents shapes as signed distance functions (SDFs). We extend DeepSDF to condition the shape generation on structural mechanics parameters, such as strain energy, load direction, volume, and dimension. We also introduce positional encoding to improve the spatial resolution of the model. Our dataset consists of various 3D shapes generated by a linear topology optimization method and Eulerian elastoplastic simulation based on the building-cube method (BCM), suitable for large-scale and high-resolution problems. We use the strain energy as a quantitative indicator of the structural performance of the shapes. We train our model on the dataset and evaluate its ability to reconstruct and generate 3D shapes that reflect the structural dynamics parameters. Our numerical results indicate that our model can produce 3D shapes with high fidelity and diversity and achieve an average reconstruction accuracy of 88.8% for the test shapes. We also show that our model can generate novel 3D shapes that satisfy the desired structural performance by manipulating the structural mechanics parameters and the latent vector. Our model and dataset open up new possibilities for 3D shape generation and structural design using deep learning.

Imaging-based methods in computational medicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DERIVING INTERVERTEBRAL DISC FEM MODELS FROM MRI IMAGE SEGMENTATION IN LARGE COHORTS

Kati Nispel[1], Tanja Lerchl[1], Gabriel Gruber[1], Hendrik Moeller[1], Veit Senner[1] and Jan S. Kirschke[1]*

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ABSTRACT

Patient-specific intervertebral disc (IVD) models for Finite Element Analyses (FEA) struggle to achieve high fidelity. Limited soft tissue segmentation methods contribute to inaccuracies in numerical models, especially in modeling IVD and vertebra contact surfaces. As a result, interindividual stress distributions and deformations are can be imprecise. In automated pipelines, which are inevitable for analyzing back pain in large cohort studies, model fidelity is even more compromised. [1]

To address this, our team has developed an innovative pipeline for automatically deriving high-fidelity Finite Element Method (FEM) models of patients' IVDs from MRI scans. This pipeline is a product of an interdisciplinary effort among medical professionals, IT specialists, and mechanical engineers. Here, we focus on the pipeline parts from the segmentation mask to the FEM model, while the segmentation method is described in detail elsewhere [2]. Based on the segmentation, surface meshes of the vertebrae and IVDs were created using the marching cubes algorithm. For this, we implemented separate smoothing pipelines for vertebrae and IVDs, which include multiple distinct steps while preserving the anatomical geometries. IVD smoothing is parted in three steps, which are (I) overall preprocessing, (II) selective smoothing and (III) postprocessing. In (II), we remesh the nodes of the IVD mesh to match the nodes of the adjacent vertebral endplate surface, ensuring the contact surface to be perfectly aligned. After smoothing, IVD surface meshes are transformed to volumes using surface reconstruction. Volumes are meshed uniformly with tetrahedral elements. We rated the performance of our pipeline by examining (I) the average processing time per IVD in 30 patients with full spine MRIs (=220 IVDs) taken from the German National Cohort (GNC) and (II) the quality of the meshes based on their aspect ratios.
On average, less than 2 minutes were needed to create one IVD model from the segmentation file. The average aspect ratio of tetrahedrons was 1.62 for all models, ensuring a suitable mesh quality for simulation.

Our pipeline enables simulation studies with varying loads in large cohorts and paves the way to creating more complex, heterogeneous IVD meshes.

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16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics

July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ERROR ESTIMATES FOR DYNAMICAL LOW RANK APPROXIMATIONS OF RANDOM PARABOLIC EQUATIONS

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ABSTRACT

Dynamical Low Rank (DLR) approximation for time-dependent problems with random parameters can be seen as a reduced basis method, in which the solution is expanded as a linear combination of a few well-chosen deterministic functions with random coefficients. The distinctive feature of the DLR method is that the spatial basis is computed on the fly and is free to evolve in time, thus adjusting at each time to the current structure of the random solution. In this talk, we consider the DLR approximation for a random parabolic equation discretized by a stochastic collocation finite element method and advanced in time by a projector-splitting scheme. Similarly to the continuous DLR approximation, our fully discrete scheme is shown to satisfy a discrete variational formulation. By exploiting this property, we derive a priori and residual-based a posteriori error estimation for a linear parabolic problem with random parameters. The error estimates consist of four terms controlling the finite element error, the time discretization error, the stochastic collocation error, and the rank truncation error. The a posteriori error estimator can be used to drive an adaptive choice of the four discretization parameters.

Current trends and advances in enriched finite element methods and coupled simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A LOW DIFFUSION VERIFIED CONFORMING TRANSIENT H-R UNSTRUCTURED ADAPTIVE MESH REFINEMENT (CTHRUAMR) METHOD FOR COUPLED INTERFACE PROBLEMS

David Noble[*1]*

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ABSTRACT

Enriched finite element methods are powerful tools for coupled multiphase and multimaterial problems with moving interfaces. To capture the discontinuities across interfaces, these methods introduce some form of enrichment of the degrees of freedom. Additional unknowns are assigned to the mesh entities (elements, nodes, sides, or edges) that are associated with these interfacial elements, and additional equations are formulated.

In CDFEM[1], level sets are used to describe the domain of each material or phase. Nodes are added at the intersection of each level set surface with the edges of the input mesh, and a conforming mesh is generated automatically. This allows the weak and strong discontinuities across the interfaces to be captured using standard finite element methods.

In recent work, a new strategy has been developed for automated interface conforming tetrahedral mesh generation, which produces higher quality discretizations than CDFEM techniques. The Conforming Transient h-r Unstructured Adaptive Mesh Refinement (cThruAMR) method uses a combination of h-adaptivity and r-adaptivity to generate high quality meshes that conform to a moving interface. The term h-adaptivity is used for refining or cutting the mesh. CDFEM uses interface-conforming h-adaptivity to capture dynamic topology problems. The term r-adaptivity is used for moving the nodes of the mesh to capture a desired feature. By combining h and r adaptivity, cThruAMR can produce high quality meshes even for dynamic topology problems. The method is closely related to the Conforming to Interface Structured Adaptive Mesh Refinement (CISAMR) method but employs a general unstructured mesh and is developed for transient moving interface problems. A new, low diffusion, cThruAMR method has been developed that has lower error than earlier implementations of the method.

This focus of this talk is the description of cThruAMR for coupled interface problems including the strategies employed for r-adaptivity, level set advection, dynamic DOF handling, and interfacial boundary conditions. The method is verified using multiple benchmark problems and is shown to produce optimal convergence rates. The discretization is shown to have better conditioning and much better mesh quality compared to CDFEM.

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Smart structures – Modelling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A STUDY ON THE STRUCTURAL SYSTEMS WITH TAPERED HARDENING-TYPE HYSTERESIS DEVICES

Aguri Noda[*1], Toshio Maegawa[1], Soma Mitsui[2] and Masamichi Sasatani[2]*

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ABSTRACT

Japanese seismic design allows for the formation of plastic hinges at the ends of beams in the event of a major earthquake. These plastic deformations in the structure increase its seismic energy absorption capacity and help prevent the building from collapsing.
However, in cases where seismic motion exceeds expectations, the seismic energy surpassing the structure's absorption capacity may cause partial destruction, ultimately leading to building collapse. Allowing for the plastic deformation of structural members may result in a lengthening of the building's natural period due to repetitive seismic motion. In such instances, prolonged seismic motions could unexpectedly damage buildings.
For this background, a structural system with hardening-type hysteresis was proposed to enhance building durability. This system consists of a moment frame connected to displacement control devices with hardening-type hysteresis. The devices prevent excessive deformation of the building in the event of seismic motion exceeding the expected level and provide the building with a margin of safety. This paper carries out experiments and analysis on the device with hardening-type hysteresis.
The device consists of steel rods, disc springs, a pair of tapered members, and a pair of up-thrust members. Specifically, the tapered and up-thrust members are connected by steel rods fastened with disc springs. It has low stiffness up to a defined displacement when compressive and tensile forces are applied. It becomes highly stiff when further forces are applied.
Firstly, to verify the fundamental properties of the device, loading tests were conducted using various specimens with different taper angles and combinations of disc springs. As a result, two levels of stiffness were obtained as expected.
Subsequently, a finite element analysis was performed under the same conditions as the experiment. The results of this analysis broadly aligned with the experimental results, confirming the capability of the finite element analysis model to replicate the experiments.
We designed a hardening-type hysteresis based on these results. The hysteresis model was applied to a multi-story steel-frame structure and subjected to seismic analysis to confirm the effects of the reduction of acceleration and deformation on the building.

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New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPLORATION OF MICROSTRUCTURES WITH NEGATIVE THERMAL EXPANSION COEFFICIENTS USING TOPOLOGICAL DERIVATIVES

Masaki Noda[*1] and Takayuki Yamada*[1]

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ABSTRACT

The application of topological derivatives in topology optimization has been a focal point in various studies. Particularly, research in multi-material topology optimization methods has progressed, yet attempts to derive microstructures with negative thermal expansion coefficients based on topological derivatives are scarce. In this study, we present topological derivatives related to thermal expansion, i.e., topological derivatives that take into account the deformation of the structure due to thermal stress at a uniform temperature change. We employ these derivatives in creating microstructures with negative thermal expansion coefficients. To derive the optimal multi-material structure, we utilize the multi-material topology optimization method previously proposed by the authors [1]. This research applies existing theories of topological derivatives [2] to a novel context, exploring new possibilities in topology optimization.

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Recent advances in meshfree and particle methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SIMULATING OVERTURNING MOMENTS AND PILE RESISTANCE CAPACITY IN TSUNAMI-EXPOSED REINFORCED CONCRETE BUILDINGS WITH MPS METHOD

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ABSTRACT

Overturning moment and foundation resistance capacity are interesting in the design of reinforced concrete (RC) buildings which are overturned by the force of a tsunami wave impact, as occurred in the 2011 off the Pacific coast of Tohoku Earthquake. Before this event, RC buildings were considered to be tsunami- and earthquake-resistant because of their large self-weight and strong outer walls. Overturning of RC buildings in Onagawa-cho, Miyagi Prefecture was determined by Nakano et al. [1] to be caused by tsunami wave overturning moment exceeding the resisting moment from the building self-weight (accounting for buoyancy) and foundation pile pull-out strength.

In our study, algorithms for computing the overturning moment, uplift moment, and resistance capacity from pile foundations, resulting from the impact of a collapsing water column on a rigid block in a two-dimensional moving-particle semi-implicit method- (MPS-) based simulation [2] are presented. The MPS method used in this study, both fluid particles and wall particles have variables of pressure to enable accurate calculation of fluid particle acceleration due to pressure gradient when in the vicinity of rigid walls. These algorithms use the pressure values from the wall particles of the rigid block to approximate combined hydrostatic and hydrodynamic pressure of the fluid on the block and the pore water pressure increase in the underlying soil. These pressure values provide a convenient simplification of both uplift and pile pull-out capacity calculations unique to the MPS method by eliminating the need for complex seepage flow simulation in the determination of water pressure in the underlying soil.

The simulation was verified using two benchmark tests: one of hydrostatic conditions and the other based on the dam break experiment by Lobovský et al. [3]. The pressure output showed good agreement with both the pressure data from that experiment and the analytical solution of hydrostatic pressure.

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Physics-informed machine learning for numerical modelling in engineering and science
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTIPHYSICS-INFORMED NEURAL NETWORKS FOR NON-DESTRUCTIVE STRUCTURAL HEALTH MONITORING IN THERMOMECHANICAL SYSTEMS

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ABSTRACT

This study introduces a model utilizing Multiphysics-informed neural networks (MPINNs) to predict full-field temperature, displacement, and stress of silicon wafers regarding thermomechanical problems. Traditional methods relied on numerous temperature sensors to detect wafer operation and defects; however, they were insufficient for monitoring the temperature, displacement, and stress fields across the entire wafer. While recent advancements in deep learning models have led to approximate models predicting outputs based on input data, there are limitations in accuracy for untrained domains due to the low precision of extrapolation of data-driven approaches. Although PINNs offer high prediction accuracy even in data-absent areas due to their integration of physical knowledge; they require retraining when boundary conditions or loads change. To overcome these challenges, this study incorporated temperature data from a limited number of sensors into the input layer of existing MPINNs and trained them under various loading conditions. Consequently, it was observed that using this sparse temperature data alone accurately predicted the temperature, displacement, and stress across the entire domain. Furthermore, various techniques such as sequential training and model parameter sharing were quantitatively analyzed to enhance the convergence of MPINNs.

Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTI-TRACK AND MULTI-LAYER SIMULATION METHODOLOGY FOR POWDER BED FUSION PROCESS BY LATTICE BOLTZMANN AND MULTI-PHASE FIELD METHODS

Sukeharu Nomoto[1], Jun Katagiri[1], Masahiro Kusano[1], Tomonori Kitashima[1] and Makoto Watanabe[1]*

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ABSTRACT

A three dimensionally integrated numerical framework using lattice Boltzmann method and multi-phase field method is proposed for simulating melting and solidification of metal alloy in laser powder bed fusion process. Modified lattice kinetic scheme that is a kind of lattice Boltzmann method is applied to simulate fluid flow consisting of atmosphere gas and melt liquid with free surface. Melting and solidification of metal alloy are modelled by multi-phase field method with consideration of grain interface anisotropy. Conserved Allen-Chan equation, which is also transformed to the modified lattice kinetic scheme formulation, is adapted to track the liquid-solid free surface moving dynamics. Thermal equation with heat source of traveling laser beam is solved by coupling fluid flow and melting / solidification analysis. Highly parallelized computational program is developed by using MPI and OpenMP hybrid method. A three-dimensional model of powder bed fusion additive manufacturing of Ni alloy is built by consisting of atmosphere gas, base plate, and powder regions. The base plate is modelled with multi-grains generated by Voronoi tessellation method, of which crystalline directions are randomly distributed. Ni alloy powder, of which particle assumed sphere, is set by discreet element method. Seamlessly analysis from melting to solidification is performed in condition of two laser beam tracks and two powder layers. Solidification microstructure constructed with epitaxially multi-grain growth is formed. The obtained result is qualitatively compared with experimental measurement. It is confirmed that the present numerical framework gives us high speed and robust method for large scale model of powder bed fusion process.

Computational methods in environmental fluid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ON THE NEED FOR THE INERTIAL EFFECTS FOR EVALUATING THE MITIGATION PERFORMANCE OF THE COASTAL TREES IN 2D UNSTEADY TSUNAMI FLOW SIMULATIONS

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ABSTRACT

2D nonlinear shallow water (SW) simulation is a common way to evaluate tsunami propagation and inundations in the fields of coastal engineering. There are many open-source software or in-house codes that can simulate how tsunamis propagate from offshore to onshore, and how they are prevented/attenuated from the coastal structures, such as seawalls or vegetation. For evaluating such the resistance effects of coastal vegetation, the source terms, which represent the resistance forces against the flow, are generally inserted into the momentum equations of 2D SW equation. Although many researchers model the source term based on the idea that the resistance effects are mainly caused by the non-inertial, so-called drag effects only, Suzuki et al. 2019[1] insisted that the inertial effects would become larger inside the coastal trees. Indeed, modeling only the drag effects seemed to have a discrepancy in expressing the instantaneous amplifications of the tsunami impact as reported by Aburaya et al. 2002[2]. That is, they are required to employ a much larger drag effect parameter only in the very short term during the wavefront reaches the structures. Therefore, we shall consider the effects of inertial force in the evaluations of the mitigation performance of the coastal vegetation.

In this study, we aim to investigate how the inertial forces due to the presence of trees ultimately influence disaster mitigation performance. We first set up a 2D nonlinear SW momentum equation considering the inertial effects due to the presence of the trees in addition to the drag effect. To identify the parameter appearing in the formulation of drag/inertial forces, we preliminary carry out the 3D numerical flow tests with the open channel domain, and the tree geometry generated by the L-system[3]. From implementing the resultant parameters and the established momentum equations, we simulate the 2D unsteady flows. The comparison with 3D flow simulations with direct tree resistance provides the discussion for the necessity of the inertial effects.

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Advanced materials and smart structures: Modeling, simulation and testing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STABILIZATION OF LARGE DEFORMATION ANALYSIS FOR A NONRECIPROCAL GEL UNDER CYLINDRICAL INDENTATION

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ABSTRACT

A nonreciprocal gel is a uniform composite consisting of oriented nanosheets embedded in a hydrogel [Wang et al., 2023. Mechanical nonreciprocity in a uniform composite material, Science 380, 192–198]. This material exhibits mechanical nonreciprocity owing to buckling of nanosheets. Mechanical nonreciprocity has many potential engineering applications in energy conversion and biological manipulation [Sun and Kang, 2023. A mechanically one-way material, Science 380, 135].
In the previous study, plane-strain finite element analysis for cylindrical indentation of the nonreciprocal gel was performed to clarify the deformation mechanism. The nonreciprocity of the gel was modeled by extending the framework of orthotropic linear elasticity. Relative material constants were nonlinearized by line approximations as functions of applied strains based on experimental data, i.e., the nonreciprocity was explicitly introduced into the constitutive model. Numerical results elucidated the relationship between the nonreciprocity and the asymmetric response of the gel. It was, however, found that severe large deformation drastically degrades the robustness of the computation. Asymmetric deformation occurs due to both nonreciprocity and large compressive deformations, especially in the region just below the cylinder. It was further found that hourglass deformation modes arising in the severe deformation elements lead to this vulnerability [Nonogaki et al., 2023. Large deformation analysis of a nonreciprocal gel under cylindrical indentation. Japan Society for Computational Methods in Engineering 23, 123–128].
In this study, we demonstrate that the introduction of artificial viscosity and hourglass control stabilizes the large deformation analysis of the nonreciprocal gel. The artificial viscosity allows us to complete the computation even under severe large deformations. The hourglass control also prevents hourglass deformation modes. We study the effects of these parameters on the computational accuracy and efficiency. Using larger values of two parameters increases computational efficiency but decreases computational accuracy. Parametric studies reveal the proper range of two parameters where computational efficiency is compatible with accuracy.

Multi-scale modeling and upscaling for flow induced vibrations, from local reference simulations to certified industrial tools
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FSI SIMULATION WITH IMPOSED DISPLACEMENTS USING TRIOCFD ON A SCALE-RELEVANT MOCKUP OF A NUCLEAR FUEL ASSEMBLY

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ABSTRACT

Investigating the behavior of fuel assemblies under mechanical solicitation in a fluid flow is of key importance for the safety of nuclear pressurized water reactor (PWR) in case of seismic events. In this context, experiments have been conducted with 1:2 scale fuel assembly mockups that were forced to vibrate in an ascendant fluid flow [1]. To have a better understanding of fluid-structure interactions in such a configuration, we aim at numerically simulating the setup, and the first step for this is to develop a fluid modeling with moving boundaries. This communication presents the first fluid-structure simulation on a large and complex geometry with imposed displacements using TrioCFD [2], the open-source CFD code of CEA, and how it was modeled.

The turbulent fluid flow is modeled with a standard k-ε RANS (Reynolds-Averaged Navier-Stokes) approach. In order to reduce the computational cost, the complex geometry of the spacer grids is modeled with a porous medium where an anisotropic pressure loss is defined. In the axial direction, the latter has been calibrated to reproduce the pressure drop experimentally measured throughout the entire assembly and in the transverse direction, a larger pressure loss is imposed to mimic the displacement of the fluid due to the spacer grid structure. The moving boundaries are handled by the Arbitrary Lagrangian-Eulerian method [3] implemented in TrioCFD.

After a static computation to initialize the fluid velocity field, the dynamic computation is then realized with an imposed displacement of the assembly. This displacement mimics the first vibration mode of an Euler-Bernouilli pinned-pinned beam, with an amplitude of 1mm and a frequency of 5 Hz. The calculation of about 18 periods using a 70 million tetrahedral element mesh needed the use of about 50,000 CPU hours. This reasonable computational cost as well as the first analyses that we will present display a glimpse of a wide potential of physical parametric studies.

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Multi-scale modeling and upscaling for flow induced vibrations, from local reference simulations to certified industrial tools
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SENSITIVITY ANALYSIS FOR TURBULENT FLOWS

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ABSTRACT

Our work focuses on sensitivity analysis for the RANS equations more precisely the k− ε model, using the Polynomial Chaos Method (PCM) [1]. PCM is a probabilistic method consisting in the projection of the model output on a basis of orthogonal stochastic polynomials in the random inputs. The stochastic projection provides a representation of the model output variability with regard to the inputs.

PCM has been used for Uncertainty Quantification in many domains. It offers significant advantages in various engineering applications with turbulent flows, despite being a highly challenging problem. Due to the difficulty of applying the PCM to the k − ε [3], we first used it for the Navier-Stokes equations, which is easier to perform.

First, the first-order sensitivity of the Navier-Stokes equations using the PCM is computed. A Finite Element-Volume (FEV) [2] numerical scheme for the Navier-Stokes equations is proposed. This discretisation is integrated into the open-source industrial code TrioCFD, promoted by the CEA. The FEV method is a widely employed discretisation technique for partial differential equations. It ensures local mass conservation, which is essential for some physical issues.

Second, the first-order sensitivity Navier-Stokes equations are discretised according to the FEV. However, the most significant and original point is the discretisation of the non linear term. Then, a stability estimate for continuous and discrete Navier-Stokes equations is established. The PCM provides an estimate of the mean and the variance of the solution of the Navier–Stokes equations when there are uncertain parameters, and this estimated variance is used to compute confidence intervals.

Some numerical tests are presented to evaluate the polynomial chaos method and to compare it to the Monte Carlo and Taylor expansion methods.
Finally, we show that the standard PCM is not directly applicable to the k − ε equations but some novel works are in progress to extend this method to the turbulent flows and the first results are promising.

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Advance modeling and simulation in complex porous media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GENERATION AND QUANTIFICATION OF SYNTHETIC POROUS MEDIA

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ABSTRACT

Firstly, we introduce an innovative pipeline for the generation and permeability evaluation of synthetic porous media. Addressing the unpredictability in natural porous materials, our approach focuses on creating controlled synthetic media, essential in diverse fields such as biomechanics, industrial applications, and medical science. We explore the complexities of porous microstructures and fluid-structure interactions, employing advanced technologies like CT and micro-CT for accurate 3D microstructure analysis.

Secondly, we address the continuum biological hydrodynamics simulation in complex geometries, by utilising the Entropically Damped Artificial Compressibility (EDAC) solver for The Discretisation-Corrected Particle Strength Exchange (DC-PSE). The solver is coupled with Brinkman penalisation to add a layer of robustness when dealing with such stochastic complex geometries. The Entropically Damped Artificial Compressibility (EDAC) formulation equations are solved using the DCPSE.

Finlay, we extract RVE’s from the simulated porous medium where the the averaged permeability is evaluated under vorticity criterion.

Our pipeline facilitates enhanced research in fluid movement, heat transfer, and targeted therapeutic interventions by mimicking natural tissue conditions. This work provides a novel tool for synthetic media generation and for robust computation of permeability in porous structures, contributing significantly to technological development and medical advancements.

Probabilistic learning and constrained generative models for uncertainty quantification
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CONDITIONAL DIFFUSION MODELS FOR SOLVING PHYSICS-BASED INVERSE PROBLEMS

Assad Oberai[*1], Agnimitra Dasgupta[1], Javier Murgoitio-Esandi[1] and Harisankar Ramaswamy[1]*

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ABSTRACT

Conditional generative models aim to sample from a conditional distribution given samples from the joint distribution, which makes them particularly suitable as tools for solving inverse problems in a Bayesian setting, especially when solving the forward problem is efficient. Thus, a significant body of work exists on utilizing conditional generative models for solving inverse problems. Diffusion models—a type of generative model—are responsible for significant advances in generative artificial intelligence. This work explores the use of conditional score-based diffusion models for solving physics-based inverse problems. Using multiple challenging applications in computational mechanics involving synthetic and experimental data, this work explores the efficacy of conditional score-based diffusion models in solving large-scale physics-based inverse problems. It also contrasts their performance against conditional generative adversarial networks, another class of popular generative models. It also explores the effect of various sampling and model-related hyperparameters on performance, and the behavior of these models in different limits.

16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics

July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTI-FIDELITY MODELING VIA THE DATA GRAPH LAPLACIAN

Assad Oberai[*1] and Orazio Pinti*[1]

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ABSTRACT

Low-fidelity data is typically inexpensive to generate but inaccurate, whereas high-fidelity data is accurate but expensive. To address this, multi-fidelity methods use a small set of high-fidelity data to enhance the accuracy of a large set of low-fidelity data. In this talk, this is accomplished by constructing a graph Laplacian from the low-fidelity data and computing its low-lying spectrum. This is used to cluster the data and identify points closest to the cluster centroids, where high-fidelity data is acquired. Thereafter, a transformation that maps every low-fidelity data point to a multi-fidelity counterpart is determined by minimizing the discrepancy between the multi- and high-fidelity data while preserving the underlying structure of the low-fidelity data distribution. The method is tested with problems in solid and fluid mechanics. By utilizing only a small fraction of high-fidelity data, the accuracy of a large set of low-fidelity data is significantly improved. A Bayesian version of this approach, which allows for the quantification of uncertainty in the multi-fidelity model is also described.

A NEW NUMERICAL METHOD FOR SCALAR EIGENVALUE PROBLEMS IN HETEROGENEOUS, DISPERSIVE, SIGN-CHANGING MATERIALS

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ABSTRACT

In this talk we consider time-harmonic scalar transmission problems between nondispersive and dispersive materials with generalized Lorentz frequency laws. For certain frequency ranges such equations involve a sign-change in their principle part. Due to the resulting loss of coercivity properties the numerical simulation of such problems is demanding. Furthermore, the related eigenvalue problems are nonlinear and give rise to additional challenges. We present a new finite element method for such problems, which is based on a weakly coercive reformulation of the PDE. The new scheme can handle C^1 interfaces consisting piece-wise of elementary geometries. Neglecting quadrature errors the asymptotic convergence of the method follows straightforwardly. For our implementation we apply a simple, but nonstandard quadrature rule. We present computational experiments in 2D and 3D for source and eigenvalue problems, which confirm the stability and convergence of the new scheme.

Physics-based data-driven modeling and uncertainty quantification in computational materials science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODEL VALIDATION VIS À VIS PREDICTIVE CAPABILITY

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ABSTRACT

Simulation is becoming the primary tool in predicting the performance, reliability, and safety of engineered systems. Terminology such as “virtual prototyping,” “virtual testing,” and “full physics simulation” are extremely appealing when physical testing, budgets and schedules are highly constrained. When pressure from competitors or upper management is added, project managers are persuaded to rely heavily on simulation for decision making. Many contend that higher fidelity physics modeling, combined with faster computers, is the path forward for improved predictive capability of systems. However, when you examine the rate of increase in physical complexity, computational requirements, and system information requirements when finer scales of physics are included in modeling, the argument for increasing predictive capability is questionable.

This presentation takes the perspective of the decision maker, project manager, or regulatory authority who is accountable for their decisions on engineered systems. It is pointed out that this perspective is in sharp contrast to a researcher or academic involved in developing mathematical models and computational methods for simulation. I use the concept that model validation is the assessment of model accuracy determined by comparison with experimental measurements. I define predictive capability as the estimation of the total uncertainty in any system response quantity of interest, regardless of whether it relates to system performance, reliability or safety. Predictive capability is the emerging field attempting to capture all aspects of uncertainty in order to foretell the response of a system for conditions where no experimental data are available. I argue that estimation of predictive capability is the most constructive and prudent path forward from the perspective of the decision maker or regulatory authority. In contrast to traditional uncertainty estimation, specifically Bayesian estimation, predictive capability attempts to capture all potential sources of uncertainty. These include model input uncertainty, model form uncertainty, and numerical solution error, as well as uncertainty in the environments and scenarios to which the system could be exposed. This talk will briefly review uncertainty quantification approaches that have been developed in fields such as nuclear power reactor safety, civil engineering and nuclear weapons. An important distinction is made between uncertainties that are random (aleatory uncertainties) and those that are due to lack of knowledge (epistemic uncertainties). I argue that imprecise probability approaches offer the most appropriate description to represent the total predictive uncertainty for a decision maker. This presentation also points out the organizational/customer resistance to improved estimation of predictive capability.

Geomechanics of the cryosphere
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING SEA ICE DYNAMICS WITH A DISCRETE ELEMENT METHOD: AN OVERVIEW OF THE DEMSI PROJECT

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ABSTRACT

The Arctic has undergone significant changes in recent decades, with substantial reductions in sea ice extent and multiyear ice, leading to thinner ice that is susceptible to breakup [1]. As sea ice deforms it can fracture and create areas of open water called leads. The opening of leads exposes ocean water to the atmosphere, providing an opportunity for ocean-atmosphere energy exchange. When thermodynamic conditions are right, the water in a lead can refreeze and when compressed the ice can create a pressure ridge. These local processes, while difficult to describe, are important components of sea ice models and Earth System Models (ESM) and are challenging to reproduce with continuum sea ice models. In this talk we present a new discrete element model for sea ice (DEMSI) and discuss an overview of some of its main features including a bonded particle model, pressure-ridging contact model, particle interpolation and remapping, and sea ice thermodynamics [2]. Sea ice simulations of the Arctic Basin using DEMSI will be presented as well as a regional scale example in the Beaufort Sea north of Alaska. Simulated ice motion results will be compared with satellite observations and discussed.

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Numerical modelling of composite materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CORNER SUPPORTED THICK LAMINATED COMPOSITE PLATES

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ABSTRACT

In this study, a Ritz method-based solution of the corner supported thick Laminated Composite plate under uniform loading is presented. The flexural and shear behavior of thick laminated plates is described by five coupled partial differential equations, derived based on the “Rissener-Mindlin plate theory”. These equations have been analytically solved by many researchers for specially stacked laminated plates with simple boundary conditions and geometries. Especially for the case of arbitrary stacked thick laminated plates, the form of governing equations is too difficult to be solved by classical methods. The difficulty of the solution is further increased if boundary conditions involve free edges and corner supports. Therefore, this research is destined to develop a robust method to handle such a complicated problem. The proposed method is based on an automated Ritz method capable of yielding accurate solutions for a uniformly loaded corner-supported thick laminated composite rectangular plate having a general stacking sequence. In the proposed approach, Ritz method is cast in a matrix form and an automated symbolic integration procedure is used to allow the use of many approximating polynomial terms as required for convergence. The accuracy of the proposed method is validated by comparing the results obtained against those finite element method (FEM) solutions generated using the commercial software COMSOL Multiphysics.

Advanced discretization schemes and solution strategies for computational structural dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HIERARCHIC REISSNER-MINDLIN SHELL FORMULATIONS FOR EXPLICIT DYNAMIC ANALYSES

Bastian Oesterle[1], Rebecca Thierer*[2], Lisa-Marie Krauß[2] and Manfred Bischoff[2]*

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ABSTRACT

The hierarchic concept for structural element formulations has been developed within the group of the authors with a focus on shear deformable Reissner-Mindlin shell formulations, as can be seen for instance in [1, 2]. Via reparametrization of the kinematic variables, these formulations possess distinct primary variables for transverse shear. This directly results in element formulations that are intrinsically free from transverse shear locking. That is, transverse shear locking is avoided a priori, independent of the utilized discretization scheme.

In addition, the hierarchic structure can be exploited towards an intrinsically selective mass scaling (ISMS) scheme [3]. That is, the high shear frequencies, which usually limit the critical time step in explicit analyses using shear deformable shell elements, are scaled while the low bending frequencies remain mostly unaffected. This stands in contrast to conventional rotational mass scaling for shear deformable elements with rotational degrees of freedom, where the total rotational inertia is scaled and, therefore, also bending frequencies and angular momentum are manipulated.

In this contribution, we present recent investigations on ISMS for hierarchic plate and shell formulations. We discuss the effects of transverse shear parametrization in several transient problems with respect to efficiency and accuracy.

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Microstructures of chemically complex materials and their impacts on material properties from multiscale simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ATOMISTIC SIMULATION OF CHEMICAL ORDERING IN MEDIUM ENTROPY ALLOYS DRIVEN BY NEURAL NETWORKS: FORMATION KINETICS AND IMPACT ON MECHANICAL AND DIFFUSION PROPERTIES

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ABSTRACT

The formation of local chemical order in medium-entropy alloys and high-entropy alloys (MEAs/HEAs) has been strongly suggested in recent experimental observations and theoretical studies. Since chemical order can lead to changes in mechanical and functional properties, tailoring of chemical order is a promising approach for further improving those properties of MEAs and HEAs. However, details regarding the atomic structure of the chemical order and its formation kinetics remain unclear. In the present study, utilizing the newly developed ANNP (artificial neural network potential)-driven atomistic simulation, such as artificial-neural-network-accelerated kinetic-Monte-Carlo (ANN-kMC) vacancy diffusion simulations for vacancy jump, we first precisely depict the genuine chemical ordering structures relative to annealing temperature and duration in CrCoNi MEA. Following this, we analyze its impact on deformation/strength and interstitial/vacancy diffusion in CrCoNi MEA using ANNP-driven molecular dynamics and ANN-kMC simulations, revealing a clear link between the degree of chemical ordering and the strength and diffusion kinetics.

Modeling and simulation of coupled processes in geological media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL ANALYSES OF COUPLED THERMAL-HYDRAULIC-MECHANICAL-CHEMICAL PROCESSES WITHIN FRACTURED ROCKS BASED ON EXPLICIT FRACTURE MODELS

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ABSTRACT

For investigating the capability of a geological disposal facility for high-level radioactive waste (HLW), long-term alteration in the permeability distribution within the rock mass that work as the natural barrier, must be predicted by using the numerical simulation.
Within the natural barrier, the rock fracture generation during the excavation of the disposal cavity bring about the enhancement of permeability around the excavated cavity. And afterwards, permeability of generated fractures during excavation, may be changed by the influence of coupled processes between the various physical/chemical phenomena induced by rock fracture network, such as heat transfer, fluid flow, stress/deformation, solute transport, and the geochemical reactions of minerals and groundwater (e.g., pressure dissolution, free-face dissolution/precipitation) after disposal of HLW into the excavated cavity. Therefore, both of the rock fracture generation process and the subsequent coupled thermal-hydraulic-mechanical-chemical (THMC) processes on the generated fractures, must be resolved realistically. To resolve such processes as realistically as possible, the numerical simulator should be based on explicit fracture models. However, the most of the existing coupled THMC simulators handle the rock fractures based on the implicit fracture modeling and they cannot resolve the details of fracture generation and coupled THMC processes acting on generated fractures.
Thus, in this study, we proposed a novel coupled THMC simulator based on explicit fracture models to resolve the details of the processes from fracture generation to subsequent coupled THMC interactions. Then, the proposed simulator was validated by replicating the results of in-situ experiments such as observed trends of rock fracture generation during cavity excavation and measured permeability evolution around cavity with time after excavation. Subsequently, the simulator was applied to predict the long-term change of the permeability distribution within the natural barrier when implementing geological repository of HLW.

Advances in multi-scale, multi-material, and multi-component Topology Optimization
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PROPOSAL OF A MULTI-MATERIAL TOPOLOGY OPTIMIZATION FOR MICROSTRUCTURES USING THE ALTERNATING ACTIVE-PHASE ALGORITHM

Shun Ogawa[1], Kazuo Yonekura[1] and Katsuyuki Suzuki[1]*

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ABSTRACT

This paper introduces a method for optimizing microstructures of multiple materials through topology optimization. With a focus on lightweight and enhancing strength in mechanical structures, recent attention has turned to material design, especially in composite materials. However, designing structures with multiple materials, each having distinct properties, poses challenges, particularly when dealing with small-scale objects and complex mechanical behaviors. To address this, we present a multi-material topology optimization approach tailored to material design challenges. Specifically, it optimizes the arrangement of multiple materials in the microstructure using an isotropic elastic model and tackles the synthesis maximization problem of the macrostructure composed of these microstructures. A decoupling multi-scale analysis is applied in topology optimization to integrate microstructure and macrostructure.

While there are numerous reports on multi-scale topology optimization methods [1] using a single design variable, such as single-material or two-phase material approaches, challenges arise when dealing with multi-material topology optimization involving three or more phases. The complexity of managing multiple design variables and interpolating material property functions makes extending conventional topology optimization systems difficult. This complexity is further heightened in multi-scale topology optimization that couples microstructures and macrostructures.

To overcome these challenges, we apply the Alternating active-phase algorithm [2], an extension of the framework of the conventional two-phase material density method, as the topology optimization algorithm. This algorithm sequentially selects two phases from multiple materials, solving subproblems based on the topology optimization of conventional two-phase materials. Applying this operation to all materials allows us to leverage the established conventional two-phase material topology optimization system. This not only enables us to reuse insights from established methods but also provides the advantage of constructing a concise topology optimization system for complex microstructures.

The paper presents the problem formulation, sensitivity analysis, and algorithm for multi-material topology optimization based on the Alternating active-phase algorithm. Finally, several numerical examples are provided to demonstrate the effectiveness of the proposed method and highlight future works.

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NUMERICAL ANALYSIS OF CRACK PATH INSTABILITY UNDER THERMAL LOADING

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ABSTRACT

Predicting crack growth remains a significant challenge in the field of fracture mechanics. A simple experiment firstly performed by Yuse and Sano (1993) [1] has attracted many attentions due to well-controlled quasi-static crack propagation in glass plates. In their experiment, a thin glass plate was moved from a hot heater to a cold water bath at a constant velocity. At this time, an initial crack placed on the bottom of the glass plate propagated under thermal stress. The crack paths exhibited transitions of straight, oscillating, and branching cracks depending on factors such as quenching speed, temperature difference between the heater and the water bath, and/or the width of the glass plates. Despite the simplicity of the experiment, the mechanism behind the transition of crack paths remains unexplored.

This research focuses on simulating crack path transitions in quenched glass plates to analyze the relationship between the thermal stress field and crack path instability. We implemented a technique to incorporate the thermal stress field into Particle Discretization Scheme Finite Element Method (PDS-FEM) for thermal crack analysis. In the simulations, we prepared 2D analysis model and varied quenching speed and width of the glass plate. Our simulation results successfully reproduced the transitions of the crack paths, including straight, oscillating, and branching cracks. Also, we show interactions between changes in the thermal field and the crack growth. We ensure that these results will contribute to an understanding of the mechanism of the mechanisms behind crack path instabilities.

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SYMBOLIC REGRESSION BASED ON BAYESIAN INFERENCE AND ITS APPLICATION TO ADDITIVE MANUFACTURING

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ABSTRACT

Symbolic regression (SR) has gained attention in scientific research due to its intrinsic interpretability. SR commonly employs genetic programming (GP) to explore the model search space. GP serves as a global optimization technique designed to prevent convergence to local optima but faces challenges, including equation bloat, overfitting to sparse or noisy datasets, and convergence speed. To address these challenges, SR has incorporated Bayesian inference. In this study, we introduce Markov chain Monte Carlo Symbolic Regression (MCSR), where SR integrates the Markov chain Monte Carlo (MCMC) method. In MCSR, we use the categorical distribution to represent the likelihood of selecting mathematical operators at each node within an acyclic graph. MCMC functions as the evolution algorithm in MCSR, aiming to discover the optimal categorical distribution that accurately depicts the training dataset. The MCSR algorithm comprises five consecutive steps. (1) an initial population of weight tensors is generated using the standard normal distribution, (2) candidate weight tensors are generated using the Gaussian distribution, (3) categorical distributions are calculated, and acyclic graphs are sampled from these distributions, (4) the population of the next generation is selected between the current and candidate weight tensors using rejection sampling, and (5) the second to fourth steps are iterated until any weight tensor in the population satisfies the user-defined threshold. The robustness of MCSR to overfitting given noisy datasets will be demonstrated through various benchmark problems. Lastly, we illustrate the utility of MCSR in scientific or engineering research. For instance, we demonstrate how MCSR can be applied to construct a surrogate model for topology optimization. Additionally, we will demonstrate that MCSR can be utilized to learn a mathematical model representing the relationship between the cooling rate and input values in additive manufacturing, such as laser power and velocity.

Complex fluid flows in engineering: Modeling, simulation, and optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VORTEX GENERATION IN THE FEED SLOT DURING SLOT COATING

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ABSTRACT

Slot coating is a major technique employed during the coating of battery slurry electrodes, necessitating a uniform and stable product. Preventing various defects that may arise during the slot coating process is crucial. In particular, vortex formation in the feed slot can lead to critical defects. Vortices in the feed slot can cause unpredictable flows due to the coagulation of slurry particles or the leakage of large particles, resulting in the unevenness of the final product.

This study focuses on quantifying the vortex generated in the feed slot during slot coating and analyzes how its location and size change under varying process conditions. The trends were examined by altering geometry and process parameters, comparing the effects of two types of fluids – Newtonian and Carreau fluid - for analyzing the impact of shear-thinning characteristics. Finite Element Method-based computational simulations were employed for flow simulations, and clustering techniques were applied to stream function data for vortex quantification.

The analysis of the influence of geometry parameters revealed that, in comparison to the coating gap, an increased feed slot height tends to promote the generation of feed slot vortices. From a process parameter perspective, it was observed that higher substrate speeds relative to the flow rate result in the enhanced formation of feed slot vortices. Lastly, the study confirmed that shear-thinning characteristics inhibit vortex formation. The findings provide insights into optimizing the coating process and mitigating issues about the vortex.

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Current trends and advances in enriched finite element methods and coupled simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE MODELING OF LOCALIZED DAMAGE IN CERAMIC MATRIX COMPOSITE STRUCTURES WITH THE GENERALIZED FINITE ELEMENT METHOD

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ABSTRACT

Ceramic Matrix Composites are showing promise as a structural material in high-speed aircraft. These materials have excellent strength-to-weight ratios and are resilient in the extreme environments encountered with high-speed structures. High-speed structures have complicated loading and structural features that shrink the structural length scale. CMCs bring several relevant length scales considerably larger than traditional metals, especially when modeling material failure. As the structural and material length scales approach each other, fundamental assumptions of homogenization theory are no longer valid. This requires a more rigorous, and significantly more expensive, analysis of the structure. However, this convergence of length scales typically occurs in localized areas of the structure: around sharp loads, high-gradient temperature profiles, connections, material interfaces, etc. A multiscale method based on the Generalized Finite Element Method with global-local enrichment functions (GFEMgl) is used to incorporate the local structural features, relevant material microstructure, and nonlinear constitutive behavior at these hot spots into global structural behavior on the fly. The proposed method can make use of homogenized material models throughout the majority of the structure, where there is sufficient separation of length scales. A damage model formulated to capture CMC failure modes at an intraply level is used to capture the nucleation and progression of damage in structural hot spots where homogenization theory is not valid. The method is shown to capture damage nucleation and progression accurately and efficiently in CMC structures when compared against industry-standard methods.

Imaging and computational methods for biomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INFLUENCE EVALUATION OF FLOW DIVERTER STENT PARENT VESSEL COVERAGE ON CEREBRAL ANEURYSM THROUGH THE CFD-DEM COUPLING SIMULATION

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ABSTRACT

A cerebral aneurysm is a type of cerebrovascular disorder characterized by the development of a balloon-like bulge in a part of the brain's arteries. When it ruptures, it can lead to subarachnoid hemorrhage, and due to the high mortality rate following onset, treatment must be initiated before the cerebral aneurysm ruptures.

To address this, the Flow-diverter Stent (FDS) placement has been developed specifically for large cerebral aneurysms. In this procedure, a device known as FDS, consisting of a cylindrically woven metal wire, is utilized. The FDS is placed in the neck of the cerebral aneurysm from within the blood vessel using a catheter for treatment. The embolization process gradually reduces the blood flow velocity entering the cerebral aneurysm, and endothelial cells invade the surface of the FDS, eventually closing the gaps between the struts and occluding the cerebral aneurysm.
Ensuring effective treatment outcomes in cerebral aneurysm treatment with FDS requires precise placement of the FDS. Improper placement may result in increased blood flow velocity and Wall Shear Stress (WSS) within the cerebral aneurysm or elevated pressure inside the aneurysm. Such phenomena suggest a potential risk of rupture, especially in the case of giant aneurysms.
Considering these circumstances, in this paper, we evaluated the impact of FDS placement on cerebral aneurysms by creating multiple FDS placement models with varying proximal and distal positions within the aneurysm. Subsequently, we conducted fluid-structure coupled analysis using the Particle Finite Element Method (PFEM) for the blood and the Discrete Element Method (DEM) for the FDS, comparing the behavior of blood and evaluating WSS and pressure inside the cerebral aneurysm based on the placement of FDS. The results of these analyses are presented.

Recent advances on interfaces dynamics modeling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL ANALYSIS OF WRINKLE TRANSFORMATION DUE TO WATER SURFACE TENSION

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ABSTRACT

Electrocapillary deformation of soft solids has received growing attention in both fundamental research and technological applications [1]. Recently, researchers have experimentally observed capillary-induced transformation of wrinkles in bilayers composed of a thin film on a soft substrate [2]. When a water droplet comes into contact with a pre-wrinkled hydrophilic surface, water filaments instantaneously develop around the contact line. This transformation results in the emergence of folds that resemble biological patterns. Since film–substrate bilayers are ubiquitous in organisms where water is a major constituent, the capillary-induced wrinkle transformation could be exploited to help rationalize morphogenesis. However, the underlying mechanisms have not been fully elucidated.

In this study, we numerically investigate the water-induced morphological transformation of wrinkles to folds in film–substrate bilayers. Finite element analysis was performed under plane strain conditions using a model composed of a linear elastic film on an incompressible neo-Hookean hyperplastic substrate. Point loads corresponding to the forces generated by the surface tension of water were applied to the wrinkles to induce the transformation into folds. The critical conditions for the occurrence of the transformation and the resulting fold geometry were explored. In particular, the effects of the wrinkle aspect ratio (amplitude/wavelength), elastic modulus ratio between the film and substrate, film thickness, and surface wettability were investigated. Our results show that as the surface hydrophilicity and the wrinkle aspect ratio increase, water filaments are more likely to be generated. Furthermore, the spacing between the resulting folds can be controlled by adjusting the values of the aforementioned factors. These findings would help better understand the mechanisms of the capillary-induced wrinkle transformation.

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Data-driven methods for modeling complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN MODELS IN VISCOELASTIC FLUID FLOWS

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ABSTRACT

Viscoelastic fluids, characterized by a combination of viscous (liquid-like) and elastic (solid-like) attributes, are an important class of non-Newtonian materials. Their complexity properties find applications across various domains, leading to widespread use of computational methods to address viscoelastic fluid flows. These computational approaches have significantly contributed to our understanding of non-Newtonian mechanics. Despite advances in scientific computing for modeling and simulating viscoelastic fluid flows, many problems remain computationally challenging, such as resolving viscoelastic instabilities and elastic turbulence. Therefore, it is essential to develop enhanced numerical schemes for non-Newtonian fluid mechanics based on machine learning algorithms and data-driven strategies.

This work leverages the Sparse Identification of Nonlinear Dynamics (SINDy) algorithm to develop interpretable reduced-order models for viscoelastic flows. In particular, we explore a benchmark oscillatory viscoelastic flow on the four-roll mill geometry using the classical Oldroyd-B fluid. The chosen flow scenario encompasses canonical challenges associated with non-Newtonian flows, featuring transitions, asymmetries, instabilities, and bifurcations arising from the interplay of viscous and elastic forces.

Our approach first showcases the effectiveness of the data-driven surrogate model in predicting transient evolution and accurately reconstructing the spatial flow field for fixed flow parameters. After this, we develop a fully parametric, nonlinear model capable of capturing dynamic variations as a function of the Weissenberg number (Wi) which is related to the elastic contribution in the flow. While the training data predominantly focuses on a limit cycle regime for moderate Wi, our results demonstrate that the parameterized model can effectively extrapolate, accurately predicting dominant dynamics even in scenarios with high Weissenberg numbers.
The proposed methodology represents an initial step in the field of reduced-order modeling for viscoelastic flows with the potential to be further refined and enhanced for the design, optimization, and control of a wide range of non-Newtonian fluid flows using modern machine learning and reduced-order modeling techniques.

Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DRAG REDUCTION EFFECT OF STREAMWISE TRAVELING WAVE WITH SPANWISE PHASE SHIFT IN A TURBULENT CHANNEL FLOW

Kyohei Oishi[1], Yusuke Nabae*[2] and Koji Fukagata*[1]

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ABSTRACT

Streamwise traveling wave of wall deformation has a high potential for friction drag reduction [1]. Among others, Nabae and Fukagata [2] optimized the parameters of the spanwise-uniform streamwise traveling wave using the Bayesian optimization and achieved 60.5% drag reduction in a direct numerical simulation (DNS) of a turbulent channel flow under a constant pressure gradient (CPG) condition. However, the resultant flow in their study was unstable in the sense that laminarization and re-transition to turbulence are repeated in time. In this study, to obtain a stable and high drag reduction effect, we propose a streamwise traveling wave with a spanwise phase shift. We examine its performance by DNS of a turbulent channel flow under a CPG condition at the friction Reynolds number of Re_tau = 180. By introducing such spanwise variations to the streamwise traveling wave, we expect that the flow reversal in the near-wall region that triggers re-transition can be mitigated. We consider eight different amplitudes of the spanwise phase shift, x_off. The DNS results show that the flow remains unstable for relatively small phase shift (x_off < 63); however, for x_off > 63, the flow is stabilized, while retaining a large drag reduction effect. The maximum drag reduction rate attained is 49.7% in the case of x_off = 141, which corresponds to a half of the streamwise wavelength of the traveling wave. According to the analysis of the Reynolds shear stress (RSS) in the case of x_off = 141, the turbulent RSS is significantly suppressed compared to not only the uncontrolled case but also the maximum drag reduction case in Nabae et al. [3]. Visualization of the vortical structures reveals that quasi-streamwise vortices are concentrated at specific spanwise locations, while they are substantially suppressed in other regions.

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POSITIVE PART BASED LEVEL SET METHOD FOR OPTIMAL DESIGN PROBLEMS

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ABSTRACT

In this talk, we shall discuss level set methods for optimal design problems. Typically, a method combining Hamilton-Jacobi equations with the shape derivative is well-known, as well as a method combining reaction-diffusion equations with the topological derivative. In the so-called diffusion-based level set methods with material representations via characteristic functions, the issue of sensitivities remains in terms of differentiability, at least in gradient descent methods. In this talk, positive parts of level set functions are devised as a formulation to avoid this issue, and numerical examples for optimal design problems are introduced by employing a numerical algorithm based on nonlinear diffusion equations.

Recent advances in computational fracture mechanics and failure analysis
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LINEAR ELASTIC FRACTURE MECHANICS ANALYSIS USING S-VERSION ISOGEOMETRIC ANALYSIS - CONDITIONS FOR GUARANTEE THE ACCURACY OF EVALUATES STRESS INTENSITY FACTOR

Yusuke Sunaoka[1], Yuhi Tsuchiyama[1], Takashi Kurosawa[1], Yuto Otoguro[1] and Hiroshi Okada[1]*

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ABSTRACT

In the presentation, the formulation and the numerical implementation of the s-IGA (S-version Isogeometric Analysis, see [1] for IGA) for linear elastic fracture mechanics problem are presented. S-IGA follows the idea of s-FEM (s-version finite element method [2]). IGA patches for the structure/solid as whole and for local features such as cracks are generated separately. Then, they are superposed. It is noted that modeling local features such as cracks are not an easy task in the applications of IGA because the patch structures are always hexahedrons. S-IGA enables us to build models for the structure as whole and those for local features such as crack separately. Hence, the generations of computational model with such local features became much more tractable than the IGA alone. In a similar way of the thoughts, technique such as X-IGA which is the IGA version of X-FEM was proposed (see, for example, De Luycker et al. [3]). In this paper the equation formulation of S-IGA, computations of stiffness matrices including the coupling stiffness matrix, the singular patch method that can reproduce the so-called square root singularity and the numerical implementations of J- and interaction integral methods that are suited to the IGA are introduced. Then, the condition to guarantee the accuracy of evaluated stress intensity factors are presented.

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Computational models and methods for predicting cancer progression and treatment response
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A COMPUTATIONAL FRAMEWORK FOR OPTIMIZING PERSONALIZED LOW DOSE METRONOMIC THERAPY

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ABSTRACT

Low dose metronomic therapy (LDMT) is the frequent administration of cytotoxic drugs at low doses over prolonged periods without extended breaks. LDMT has emerged as a promising cancer treatment strategy for enhancing patient's overall quality of life, due to its potential to maximize progression free survival while minimizing adverse effects. However, optimizing LDMT on a patient-specific basis remains a challenging problem. Towards this end, we are developing mathematical models to characterize the main effects of cytotoxic drugs on both tumor growth and toxicity. More specifically, we include the therapeutic effects of different modes of drug delivery, as well as directly account for treatment induced toxicity. Using these models we identified (theoretically) patient-specific regimens that can effectively induce and maintain tumor stability (in the sense of the Response Evaluation Criteria in Solid Tumors, RECIST) while keeping treatment induced toxicity below a desired threshold. We found that LDMT requires lower steady state drug concentration when compared to regimens designed for tumor eradication. For tumors with a pre-treatment volume to carrying capacity ratio (i.e., proliferation saturation index) between 0.1 and 0.2, LDMT can yield up to a 34.6% reduction in total dose. Furthermore, we used in silico experiments to illustrate the therapeutic effects of the treatment regimens identified by our models. The simulation results show that tumor control is sustained. The tumor size remains bounded between 34.3% and 172.8% of the pre-treatment volume, with toxicity maintained below the desired threshold at all times. Our study generates hypotheses that can be directly tested in experimental settings, thereby providing a computational approach for rigorously designing personalised therapeutic regimens that balance efficacy and toxicity

Predictive digital twins
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

OPTIMAL SENSOR PLACEMENT FOR STRUCTURAL HEALTH MONITORING

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ABSTRACT

Efficient structural health monitoring (SHM) relies heavily on strategically placing sensors to optimize associated costs related to sensors, data collection, transfer, and processing. Precise sensor positioning at critical points within a structure not only ensures accurate data collection but also minimizes redundancy in measurements. This strategic placement facilitates the development of computationally efficient online anomaly detection systems.

In this study, we explore the application of compressed sensing techniques for full order reconstruction from sparse measurements. Compressed sensing involves solving an under-determined system, assuming the signal to be reconstructed is either sparse or can be sparsified through transformation. Typically, a generic basis is used for representing the sparse signal, requiring the solution of an L1 optimization problem, see [1]. However, when we possess system understanding or prior information, a customized basis can be created, simplifying the optimization problem.

Our focus here is on a simply supported plate problem subjected to dynamic loads. Utilizing proper orthogonal decomposition of snapshots from numerical simulations, we create a custom basis. A QR decomposition of the matrix formed by this custom basis identifies optimal sampling locations for data collection. The results demonstrate promising outcomes, highlighting the method's ability to accurately reproduce dynamic responses with acceptable precision using a minimal number of sensors. In the domain of structural health monitoring, the meticulous positioning of sensors is paramount, directly influencing the system's capacity to safeguard infrastructure integrity. This research contributes to advancements in structural engineering and risk mitigation by emphasizing the critical role of sensor placement in enhancing monitoring capabilities.

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Physical models and reduced order models augmentation with data for physics-informed machine learning in real-world applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

REAL-TIME FORWARD AND INVERSE SIMULATIONS OF TIME-HISTORY DYNAMIC STRUCTURAL RESPONSES USING PINNS AND AR VISUALIZATION

Toko Okuda[*1] and Mayuko Nishio*[1]

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ABSTRACT

Real-time simulation to structural responses with use of extended reality (XR) technologies to visualize results of numerical calculations is expected to realize more interactive applications of digital twins. However, some numerical calculations including the time-history analysis of structural dynamic response increase difficulties of realizing real-time performance due to computational cost of numerical integration. In this study, authors focus on the application of physics-informed neural networks (PINNs) to overcome those difficulties on a real-time structural vibration analysis. PINNs incorporate physical laws represented by partial differential equations (PDE) into the loss function, allowing for synergistic integration of physical models and data-driven methods, and it can be applied to both forward and inverse problems. This paper shows predictions of dynamic displacement and bending moment of a cantilever beam in synchronization with real-world phenomena by applying the PINNs. Here, the inputs of neural network (NN) are time and beam coordinates, and the outputs are the displacement and bending moment of the cantilever beam. The loss function includes not only the mean square error term of observation data but also those for satisfying the equation of motion of damped free vibration of a continuous beam and their boundary/initial conditions. A sequential PINNs were then developed to realize the real-time simulation. PINNs trainings and predictions are performed at each time interval close to the vibration period, and the NN weights obtained for prediction in the previous time interval are carried over to the training in the next time interval. The outputs of PINNs, displacements and bending moments through the axial coordinate of the beam at time t, were converted to color contours for intuitive understanding, and then displayed in the augmented reality (AR) on the real beam. In addition, PINNs can make unknown properties included in the PDE prediction parameters at the same time in the training process. The verification for the free vibration of a cantilever beam, whose bending stiffness changes in the beam axis direction, was conducted to verify effectiveness of the sequential PINNs to simultaneously predict displacements and bending moments (forward analysis) and estimate the bending stiffness (inverse analysis). The study suggests possibility of real-time data assimilation, which might contribute to the development of digital twin technology in the future.

Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHASE-FIELD SIMULATION OF SOLUTE SEGREGATION IN A RAPIDLY SOLIDIFIED HASTELLOY-X NI-BASED SUPERALLOY DURING LASER POWDER-BED FUSION

Masayuki Okugawa[*1], Kenji Saito[1], Haruki Yoshima[1], Katsuhiko Sawaizumi[1], Yuichiro Koizumi[1] and Takayoshi Nakano[1]*

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ABSTRACT

Additive manufacturing (AM) technologies have attracted considerable attention as they allow us to build three-dimensional parts with complex geometries easily. Among the wide range of available AM techniques, powder-bed fusion (PBF) has emerged as a preferred technique for metal AM. In particular, PBFed Ni-based superalloys are desired to be applied to aerospace industries. However, solute segregations become remarkable during the process [1] and increase the susceptibility to cracking [2]. Therefore, an understanding of solute segregation is essential for the fabrication of reliable PBF-fabricated parts while avoiding cracks. In the present study, we simulated solute segregation in a conventional solid-solution hardening-type Hastelloy-X Ni-based superalloy under the PBF process by a multi-phase field (MPF) simulation using the temperature distributions obtained by a computational thermal-fluid dynamics (CtFD) simulation.

The single-track laser-beam irradiation CtFD simulation of HX was performed using a 3D thermo-fluid analysis software (Flow Science FLOW-3D® with Flow-3D Weld module). The dimensions of the computational domain of the numerical model were 4.0 mm × 0.4 mm × 0.3 mm. The beam power and scanning speed were set to 300 W and 600 mm/s, respectively. Then, two-dimensional MPF simulations with the temperature distributions obtained by the CtFD simulation were performed using the Microstructure Evolution Simulation Software (MICRESS) with the TQ-Interface for Thermo-Calc. The simulation domain was 5 × 100 μm, and the grid size Δx and interface width were set to 0.025 and 0.1 μm, respectively. The model was solidified under the temperature field distribution obtained by the CtFD simulation. The concentration distribution and crystal orientation of the solidified model were examined.

We found that the conventional MPF model can reproduce experimentally observed dendritic structures by performing a phase-field simulation using the temperature distribution obtained by a CtFD simulation of HX. The MPF simulation revealed that the segregation behavior of solute elements largely depends on the regions of the melt pool, such as the cell boundary, the interior of the melt-pool boundary, and heat-affected regions. The sensitivities of the various interfaces to liquation and solidification cracks are compared based on the predicted concentration distributions. Moreover, the feasibility of using the conventional MPF model for PBF is discussed in terms of the absolute stability limit.

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Data-driven approaches for solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DERIVATIVE-INFORMED NEURAL OPERATORS FOR BAYESIAN INVERSION OF HETEROGENEOUS MATERIAL PROPERTIES

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ABSTRACT

We consider the Bayesian inverse problem of inferring heterogenous material parameters from displacement measurements of an elastically-deforming system. The Bayesian inverse problem is challenging due to the infinite-dimensional nature of the parameter field. We present neural operator representations of parametric PDE solution operators (specifically, mappings of material property to deformation in elasticity) that also learn the Fréchet derivatives of these operators with respect to the parameter field. When trained, these derivative-informed neural operators (DINOs) enable scalable and efficient MCMC sampling methods, which employ gradients and Hessians of negative log posteriors to accelerate the sampling. The DINO can be used as a proposal mechanism in a delayed-acceptance MCMC method to obtain asymptotically exact posterior samples, or as a replacement for the PDE when its repeated solution is prohibitive. In either case, the resulting methods can obtain significantly larger effective sample sizes than existing methods, for a given compute budget. Numerical experiments involving non-destructive evaluation of materials as well as inversion of elastic parameters for the 2011 Tōhoku earthquake are presented.

The presentation is based in part on "Derivative-Informed Neural Operator: An Efficient Framework for High-Dimensional Parametric Derivative Learning" (Journal of Computational Physics, 2024), "Derivative-informed projected neural networks for high-dimensional parametric maps governed by PDEs", (Computer Methods in Applied Mechanics and Engineering, 2022), and the manuscript "Efficient Geometric Markov Chain Monte Carlo for Bayesian Inversion Enabled by Derivative-Informed Neural Operators" (2024).

New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION OF AN AIRFOIL UNDER MASS AND NATURAL FREQUENCY CONSTRAINTS USING GAUSSIAN FUNCTION PARAMETERIZATION

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ABSTRACT

Key Words: Topology Optimization, Gaussian Function Parameterization, Frequency Constrained Structures, Aerostructural Design

Topology optimization is a procedure focused on enhancing the structural efficiency of a design subject to physical constraints such as mass, stress, deflection, and frequency. This method strategically distributes material across a design domain to optimize performance. This study focuses on a modified two-dimensional NACA 0012 airfoil under prescribed flight conditions. Central to our methodology is integrating mass and minimum natural frequency constraints to enhance material distribution within this redesigned airfoil structure. Gaussian function parameterization [1] is also employed to optimally distribute the structural supports that hold the airfoil in place. We formulate the frequency constraint as a bounded eigenvalue problem involving a combination of scaled stiffness and mass matrices. To identify the lowest natural frequency, we employ the Kreisselmeier–Steinhauser (KS) aggregation function, which is applied to the set of all computed frequencies. This function is chosen for its smoothness and differentiability. Additionally, we compute frequency constraint sensitivities using an adjoint-based method for derivative evaluation applied to the KS function.

Our approach diverges from traditional methods by allowing flexibility in the placement of supports while keeping the aerodynamic load distribution fixed. In this way, we are able to optimize support locations concurrently with the internal airfoil structure, thereby improving the design's structural and aerodynamic performance. The study compares two different optimization strategies: the Method of Moving Asymptotes (MMA) [2] and the Generalized Optimality Criteria (GOC) Method [3]. We compare the performance of each optimization algorithm to gain knowledge about the ability of each method to handle this unique problem, which combines SIMP density parameters with explicit geometry parameters.

The study's outcomes illuminate the potential of this integrated approach in topology optimization, especially for structures where aerodynamic performance is as crucial as structural integrity.

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Computational models and methods for predicting cancer progression and treatment response
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTATIONAL MOLECULAR MAGNETIC RESONANCE IMAGING IN DIGITAL HEALTH AND PETRO-PHYSICS DESIGN

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ABSTRACT

Understanding of processes such as carrier mobility, electron transfer reactions, chemical reactions in fluids, electron solvation in fluids and electron attachment and localization in clusters relies crucially on the understanding of electron dynamics in fluids at the molecular level.
In this talk we present mathematical and computational concepts (generally applicable to the analysis of biological and non-biological systems) at the molecular level with special application to digital health and petro-physics design.

i. Digital health and petro-physics design can be likened to complex systems and are often dominated by large numbers of processes. For example, when deviations occur in normal human system, human disease conditions are produced. Understanding these processes is important not just in unravelling the causes of diseases, but also the manner of disease propagation and the best plan for treatment. The inadequate understanding of molecular dynamics of diseases is one reason why many diseases remain incurable and become life-threatening. Computational molecular magnetic resonance imaging now provides new ways of visualizing molecular dynamics and management of human diseases.

Currently, the available imaging equipment no longer matches the increasing number of patients requiring healthcare. The few available imaging machines are costly to maintain while financial difficulties are making acquisition of new ones nigh impossible. Obviously, experimental methods alone are no longer enough for efficient diagnosis, therapy and prognosis. These challenges may now require development of appropriate mathematical tools and sophisticated computer simulations based on the Bloch NMR flow equations to complement laboratory and clinical observations. Such mathematical techniques [1] have the potential to provide insight into the imaging of molecular interactions through the analysis of relaxation processes as observed on computational molecular magnetic resonance.

ii The mathematical technique [1] is unique, flexible, adaptable and generally applicable for the analysis of matter (physical and biological). The technique is useful to design NMR signals of different petro-physical properties such as porosity, tortuosity and relaxation rate of rocks fluid so that reservoirs comprised of mixed lithology and mineralogy can be easily evaluated. The computational tools are useful for repetitive data processing which is otherwise difficult due to hardware limitations and logistic issues.

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Novel numerical approaches for integrated disaster simulation for digital twin from living spaces to urban scales
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT OF AN UNRESOLVED CFD-BEAM COUPLING MODEL FOR LARGE SCALE TSUNAMI-HOUSES INTERACTION PROBLEM

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ABSTRACT

In this study, we have developed an unresolved coupling model based on a drag model for Computational Fluid Dynamics (CFD) and Finite Element Method (FEM) using beam element. The proposed method involves conducting structural analysis by considering the fluid forces obtained through the drag model as external forces. Simultaneously, fluid analysis is performed, taking into account apparent volume changes and alterations in the flow field around the beam element.

As a result, even in cases where the spatial resolution of the fluid is coarse concerning the dimensions of the beam element, coupled calculations based on the drag model become feasible as long as the velocity field is appropriately obtained. Consequently, this approach proves to be suitable for large scale tsunami-structure interaction problem, including the process of houses in a coastal area being washed away by a tsunami.

In the presentation, we elucidate the formulation and implementation of the proposed methodology, and present validation results regarding the fluid forces acting on beam elements subjected to unsteady free-surface flow. Furthermore, to demonstrate the utility of the proposed approach, simulation results are presented where a wooden house models is subjected to flows mimicking a tsunami, leading to their loss.

EQUATION DISCOVERY THROUGH GENETIC PROGRAMMING REFLECTING THE IMPORTANCE OF GENERATED TERMS

Kenji Ono[*1] and Kanae Shiragami*[1]

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ABSTRACT

Efforts to estimate equations from data have garnered significant attention in a data-driven context, and recently, deterministic methods employing sparse estimation have been the focus of interest. In this paper, we propose an efficient method for estimating equations by adopting an exhaustive approach using genetic programming while evolving generations, all while retaining useful partial terms for expressing the equation. In our proposed method, genetic programming generates terms of partial differential equations, and the error between the equation constructed from these terms and the data is evaluated. Even if important terms are present in the generated equation, if the candidate equation itself receives a low score, it may lead to a long computation time to obtain an optimal solution or potentially fail to find one. To address this issue, we introduce Evolutionary Feature Synthesis (EFS), which combines multiple regression. We incorporate fitness, indicating how well candidate equations match the data, as well as importance measures for individual terms in the equation, making the search more effective. As a validation step, we conducted numerical experiments to estimate the governing equation from fluid simulation data and evaluated the validity of the proposed method. The data used in our numerical simulation were generated by solving one-dimensional linear advection, non-linear advection, and diffusion equations with various initial conditions.

The proposed approach demonstrated its ability to provide appropriate partial differential equations in both cases. As a result, it was shown that the proposed method can reproduce the original equations from simulated Computational Fluid Dynamics (CFD) data without prior knowledge of fluid dynamics. Additionally, to reduce the estimation time, an investigation was conducted to determine how much data is required to accurately estimate the equations. It was observed that a significant reduction in estimation time can be achieved by using a certain amount of temporal data, and the reduction of spatial data had a phenomenon-dependent impact on estimation accuracy.

Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SEEPAGE FLOW SIMULATION USING MULTIPLE DIAMETER MODEL

Yasuaki Ono[*1], Yuichiro Kimura[1], Kyohei Ueda[2] and Ryosuke Uzuoka[2]*

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ABSTRACT

A suction-bucket is being developed as a foundation structure for a fixed-type offshore wind turbine. The suction-bucket is a cylindrical structure with a closed top surface. In the construction of suction-bucket, the bucket is submerged until the bottom edge touches the seabed. Then, seawater inside the bucket is forcibly discharged to increase a difference in hydrostatic pressure, which is called suction pressure, between inside and outside of the bucket, causing the bucket to penetrate the seabed. The bucket installed to a predetermined depth by this method can be used as the foundation structure for the offshore wind turbine facility.

The suction pressure is an important indicator in design and installation of this foundation. An excessive suction pressure causes buckling of steel structure and ground failures, while an insufficient suction pressure causes an insufficient penetration during the installation. Especially in sandy soil, seepage flow will be generated in the ground due to the pressure gradient and it makes more difficult to evaluate suction pressure. Moreover, the seepage flow may change the soil properties and cause seepage failures.

In this study, to take into account changes in the soil properties during installation of the suction-bucket and to evaluate the suction pressure properly, a coupled model has been developed by coupling discrete element method (DEM) for describing behaviors of soil particles and computational fluid dynamics (CFD) for describing the seepage flow. In general, spherical particles larger than actual soil particles are used in large-scale DEM simulations to reduce computational load. However, it is difficult to simultaneously represent changes in hydraulic properties (pore structure) and mechanical properties of soil masses constituting the ground. For example, although large frictional or rotational resistance is necessary to reproduce the porosity of loose soils, high resistance makes it difficult to change into dense soils.

Therefore, we developed a model that can simultaneously satisfy both these hydraulic and mechanical properties as a single spherical DEM particle. This model can be used to perform large-scale coupled CFD-DEM simulation with a low computational load that properly account for changes in soils. The results of verifying the applicability of this model through model experiments are reported in this presentation.

AIR-TAXI TRAJECTORY AND DESIGN OPTIMIZATION USING SURROGATE MODELS

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ABSTRACT

Urban air mobility is an emerging vision with the potential to radically transform urban transportation. The air taxi concepts that are being proposed to enable this vision are capable of vertical takeoff followed by horizontal cruising flight. The transition from takeoff to cruise is dominated by nonlinear dynamics and complex, multidisciplinary interactions. As such, this transition significantly influences both the design and the performance of the aircraft. However, the complexity of the transition trajectory makes it difficult to include trajectory optimization and analysis in the preliminary design process. We address this by creating a co-design problem, wherein the physical parameters of the aircraft are simultaneously optimized along with the transition trajectory. The co-design problem is solved by forming a gradient-based multidisciplinary design optimization (MDO) framework which contains standard aerospace disciplines (e.g., aerodynamics and structures) as well as control. We optimize aircraft trajectories by transcribing the continuous-time optimal control problem as a discrete-time nonlinear programming (NLP) problem with collocation points where the state and the control are simultaneously defined. This method, known as shooting, integrates the equations of motion over time in order to determine the state trajectories for given control inputs. During optimization, the optimizer acts as an omniscient controller by iteratively selecting controls that minimize our objective and satisfy the constraints. Within the NLP problem we include five physics-based sub-discipline models. However, some of the physical phenomena we wish to model are complex. In that case we rely upon automatic differentiation to simplify the implementation. Some of these complex models are still too computationally expensive to include, or they contain numerical singularities for certain inputs. In this case we use radial-basis functions and tensor-product splines as surrogate models which not only reduce complexity, but also maintain fidelity and increase robustness. These surrogates are trained on data that is generated offline using the original physics-based models. This novel, surrogate-based trajectory-optimization approach is fast and robust, which means that it is well suited to co-design problems where the trajectory must be optimized many times within an inner loop of a larger aircraft design problem. Additionally, by using physics-based models we can compute actual physical objectives for the trajectories (e.g., minimum energy and minimum time) as well as for the air-taxi design (e.g., minimum mass) that are of interest to industry as well as academia.

Lattice Boltzmann modelling and study of complex flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TURBULENCE SUBGRID CLOSURE FOR THE LATTICE BOLTZMANN METHOD VIA ARTIFICIAL NEURAL NETWORKS

Giulio Ortali[*1], Nicola Demo[2], Alessandro Gabbana[1], Gianluigi Rozza[2] and Federico Toschi[1]*

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ABSTRACT

This work introduces a novel approach to learning Turbulence Subgrid Closure models within the context of Lattice Boltzmann Method using physics-constrained Artificial Neural Networks.
The Lattice Boltzmann Method (LBM) is a class of computational methods, stemming from the kinetic theory of gases, used to simulate the dynamics of fluid flows at the mesoscopic level. The fluid is represented via the dynamics of a set of discrete particle distribution functions (populations). These populations evolve according to the stream and collide algorithm, where at each time step populations hop from lattice-site to lattice-site and then incoming populations collide among one another. We work in the context of 3D Homogeneous Isotropic Turbulence on a cube with periodic boundary conditions, considering a fully resolved setting, generating ground truth Direct Numerical Simulation (DNS) data, and different coarse graining factors.
We learn a novel collisional term, expressed as a correction to the BGK collisional operator, using a physics-constrained Artificial Neural Network trained on DNS data. The model comprises a standard Multi-Layer Perceptron, followed by post-processing layers enforcing mass and momentum conservation, trained on multi-step prediction.
The proposed model shows promising results, closely capturing both energy spectra and higher-order statistics of filtered DNS data compared to traditional techniques such as the Smagorinsky turbulence model. Remarkably, our approach is fully local both in space and time, leading to reduced computational costs, enhanced generalization capabilities and interpretability. Additionally, this formulation can be in principle used to learn any new collisional operator, given the proper ground truth data, and to acquire a deeper understanding in the physics of turbulent flows.

Imaging-based methods in computational medicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT OF A DEFORMATION TECHNIQUE FOR VASCULAR ANALYSIS MODELS USING VESSEL CENTERLINES

Naoya Imai[1], Chen Wang[1], Masaharu Kobayashi[1] and Marie Oshima[1]*

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ABSTRACT

In order to provide an appropriate diagnosis for unruptured cerebral aneurysms, a follow-up examination is often performed by medical images to observe growth in a size of aneurysm and changes in hemodynamic factors such as a magnitude of wall shear stress. However, since medical images taken at various times are considered different images even of the same patient, mesh generation is conducted for each geometry model to create individual analysis models. Because of different analysis models, it is difficult to compare changes quantitatively in simulations results between analysis models. Therefore, it is important to compare simulation results with the same number of mesh elements and nodes.

In this study, we develop a method to transform the analysis model into a target one using centerlines. The method consists of five steps. In the first step, the three-dimensional vascular models served as standard vascular model as well as target ones are segmented and constructed from medical images taken at different times. In the second step, the centerlines of both models are extracted[1]. In the third step, the analysis model of standard vascular model is created by using Gmsh[2], which is a three-dimensional finite element mesh generator. The fourth step provides the information on connection between centerline and surface triangular meshes. In the final step, the target analysis model is created by transforming the centerline of the standard analysis model into that of target analysis model by applying transformation matrix between standard and target ones. The surface of target analysis model can be also transformed using connection information of centerline and surface triangular meshes. The smoothing method is also developed to smooth distorted surface meshes[3].

The verification and validation of the present model was conducted using the simple geometry. The present method was also applied to patient-specific simulations of femoral artery, in which CT images were taken at three different bending angles. The geometry and the simulation results were compared between three cases.

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Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FLOW SIMULATION BASED ON THE IMMERSED-INTERFACE APPROACH OF MULTIPHASE, COMBUSTION FLAME AND WALL BOUNDARY

Nobuyuki Oshima[*1], Nobuto Nakamichi[1] and Younghwa Cho[1]*

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ABSTRACT

A most typical target of flow simulation is to get a solution under the boundary shape of fluid, which may be given by the wall-boundary or interactively solved as the phase interface. It becomes difficult as the shape or dynamics of boundary becomes complex. In order to treat the complex interface problem, level-set approach is a useful mathematical tool, where a volume profile of scalar function defines the interface as similar as physical solution of fluid flow variables.

Oshima [1] has mathematically examined the conservation law equation governing the fluid interface assuming a combustion flame and a phase interface and related them to the viscosity solution of the level-set equation. It is shown that the phase field approximation of the non-equilibrium phase boundary and the flamelet approximation of the combustion field can be derived. These are formalized by differential equations associated with physical conservation laws derived from the principle equations for the macroscopic behavior of the fluid interface, with additional steps (e.g. reinitialization of the level-set solution) and special By constructing the discretization formula without using numerical approximation (for example, artificial viscosity by upwind difference), mathematical analysis of the accuracy and stability of the numerical method based on this has become easier.

Next question is “Can we assume a principle equation that satisfies a continuous physical solution of solid wall boundary with the modeling resolution?”. Furthermore, looking at the development of model-based design (MBD), which attempts to construct a unified methodology by digitizing everything from design concepts to performance prediction, manufacturing methods, and product evaluation, Discretization of solid boundaries also requires a systematic research method supported by universal mathematical foundations. Oshima [2] has proposed a kind of its answer as the following equation system, where a fluid occupancy function defines the solid wall boundary.
These immersed-interface approaches make us essentially free from a “grid-generation” which may insists a huge efforts of engineering simulation. This research introduces several examples in two/three-dimensional, steady/unsteady solutions applied to multiphase flow, combustion flame and wall boundary problems.

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Advances in damage & fracture modeling of multiphysics materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING SHORT CRACK PROPAGATION IN 3D POLYCRYSTALLINE MICROSTRUCTURES UNDER CYCLIC LOADING USING ADAPTIVE CRACK INSERTION

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ABSTRACT

In this study, we present a computational framework for simulating microstructurally short crack propagation in three-dimensional polycrystalline microstructures subjected to fatigue loading. Fatigue initiation process that broadly consists of nucleation of a short crack and growth of the short crack until the crack reaches sufficient length to grow based on Paris's criterion. Under certain loading conditions, fatigue initiation life could take a very substantial part of the overall fatigue life. Currently, fatigue initiation prediction models rely on the idea of tracking a fatigue indicator parameter, which does not explicitly account for short crack growth.

The proposed framework integrates a texture-dependent crack propagation criterion, crystal plasticity finite element modeling, and an adaptive crack insertion technique. We address two primary challenges that are present particularly in the context of modeling 3D short crack growth: firstly, the implementation of a distance-based smoothing technique to mitigate stress and strain oscillations at the crack tip, and secondly, the use of an adaptive local smoothing mechanism during each growth step to minimize error accumulation. The efficacy of each component of the proposed framework is detailed and tested. The proposed framework is constructed in a modular fashion such that different and material specific propagation criteria could be incorporated. Numerical investigations indicates that the proposed framework could efficiently simulate short crack growth until fracture in both full 3D and quasi-2D polycrystalline microstructures, capturing the phenomena of crack tilting and twisting, which are prominent in experimental observations of 3D crack growth. The proposed short crack propagation framework contributes to the understanding and prediction of short crack growth in polycrystalline materials.

Architected materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING OF SOFT MULTISTABLE STRUCTURES

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ABSTRACT

Reconfigurable structures, soft materials, and metamaterials have introduced new opportunities for mechanical computation, control complexity reduction, and shape programmability. Recently, architecture materials composed of patterned arrays of bistable units have gained interest due to their capabilities of exhibiting multiple energy minima, unit activation path dependency, and influence of local prestress in its global shape. As each unit cell can be reversibly inverted at a local scale, multiple stable shapes at a global scale are achieved. These shapes are highly dependent on the unit geometry, inversion sequence, number of units, and unit spatial distribution, which makes their behavior challenging to analyze and predict. Given this, simpler yet robust models need to be utilized to predict the final state of the structure, enabling faster analysis for inverse design.

This work presents a lumped-element model to determine the final shape of our metastructure in terms of the number of units, spatial distribution, and unit cell geometric parameters. We explore the effect of interrelations between units and their spatial arrangement in our metastructure's global stable shape, enabling us to target specific target positions. We further examine the interaction between units and their role in generating geometric frustration within the structure and allowing us to determine optimal strategies to leverage all these multiple states in applications such as soft robotics and mechanical computation. This opens a route for the fast design of multistable soft robots and shapes targeting of soft metastructures.

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Model order reduction for parametrized continuum mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

REDUCED-ORDER MODELING WITH AND WITHOUT LINEARIZED ADJOINTS

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ABSTRACT

Reduced-order modeling entails identifying a low-dimensional collection of variables that can be used to reliably predict a system's response or output. Techniques such as Randomized Singular Value Decomposition (RSVD), active subspaces, Balanced Proper Orthogonal Decomposition (BPOD), and the recently introduced Covariance Balancing Reduction using Adjoint Snapshots (CoBRAS) rely on adjoints to extract these variables efficiently. Since the adjoint is often difficult or impossible to access in practice, we study the extent to which adjoints are required, and what types of prior information allow us to avoid accessing the adjoint in the simplified setting of linear operator learning. While our analysis shows that some information about the adjoint is required, this information can come from prior knowledge about the operator's properties rather than direct queries to an adjoint solver. For nonnormal elliptic PDEs, we show that regularity properties provide useful information that can be leveraged to construct low-rank approximations with guaranteed accuracy from queries to the forward solution operator only. The queries are constructed using eigenfunctions of a prior self-adjoint operator such as the Laplace-Beltrami operator (LBO). Intuitively speaking, the smoothing properties of the solution operator limits the system's sensitivity to high-wavenumber inputs. Specifically, if elliptic regularity guarantees that solutions of the adjoint equation would have k weak derivatives in L^2 and the spatial domain has dimension d, then our approximation of the solution operator based on queries using the leading n eigenfunctions of the LBO has asymptotic error $\mathcal{O}(n^{-k/d})$ with respect to the operator norm. We demonstrate this approach numerically by constructing low-rank approximations for solution operators of an advection-diffusion equation ($k=2$) with space dimension $d=1$ and for linear elasticity problems ($k=2$) with space dimensions $d=2$ and $d=3$.

Phase-field modeling: Analytics, benchmarks, and discussions
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHASE-FIELD MODELING OF ELASTIC MICROPHASE SEPARATION

Hamza Oudich[*1], Pietro Carrara[1] and Laura De Lorenzis[1]*

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ABSTRACT

Spinodal decomposition is a process where an initial homogeneous but unstable mixture spontaneously separates
into two or more stable phases with a distinctive arrangement termed spinodal structure. This process can be modeled with the Cahn-Hilliard equation [1] which is based on the definition of a chemical energy density depending on an order variable, i.e. the phase field, representing the smooth transition between the unstable initial mixture and the stable phases. Spinodal structures are characterized by a length scale that, if no competing processes are accounted for, coarsens over time until complete segregation of the stable phases. Recent studies suggest that for certain mixtures involving a solid matrix, the elastic parameters of the matrix govern the coarsening stage and can even arrest it, a phenomenon that is denoted as elastic microphase separation [2].

In this work, we propose a phase-field model that captures the main features of elastic microphase separation observed in [2]. We extend the Cahn-Hilliard free-energy functional [1] to include the elastic strain energy density as well as an additional coupling term. The model is first investigated in 1D and the results show that the mechanical deformation controls both the composition of the stable phases and the initial characteristic length of the spinodal structure. Moreover, we numerically show that the proposed coupling is able to predict the arrest of the coarsening phase at a length scale controlled by the model parameters. The formulation is then extended to the multi-dimensional setting and compared to experimental results. The numerical results show excellent agreement with the experimental evidence, especially in terms of initial and arrested pattern morphology.

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Certification of simulations and model adaptation in computational science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CONCERNING ADAPTIVE REFINEMENT FOR FEM APPROXIMATIONS OF MULTIPLE EIGENVECTORS OF SCHROEDINGER-TYPE OPERATORS

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ABSTRACT

Techniques for a posteriori error estimation and adaptive algorithms for clusters of eigenvalues and their associated invariant subspaces have received significant attention over the 15 years. The general consensus is that, regardless of the particular error estimation technique and/or marking strategy, the goal of an adaptive step is not necessarily to reduce the approximation error associated with the current computed eigenbasis, but rather to reduce the error associated with its span. Independently, but over roughly the same period, significant advances have been made in the understanding of eigenvector localization, i.e. the strong concentration of the "mass" of some eigenvectors in relatively small portions of the domain, for Schroedinger-type operators. Spatial localization of such eigenvectors implies similar spatial localization of associated wave phenomena, and this has practical applications in the design of materials and structures. In this talk, we bring together these two threads of research, presenting a non-standard adaptive approach in this context that provides surprisingly(?) good performance.

Mathematics and algorithms for predictive digital twins (DT)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SURROGATE-BASED PARTITION METHODS FOR INTERFACE PROBLEMS

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ABSTRACT

Partitioned methods for coupled problems rely on data transfers between subdomains to synchronize the sub- domain equations and enable their independent solution. By treating each subproblem as a separate entity, these methods enable code reuse, increase concurrency and provide a convenient framework for plug-and-play multiphysics simulations. However, accuracy and stability of partitioned methods depends critically on the type of information exchanged between the subproblems. The exchange mechanisms can vary from minimally intrusive remap across interfaces to more accurate but also more intrusive and expensive estimates of the necessary information based on monolithic formulations of the coupled system. These transfer mechanisms are separated by accuracy, performance and intrusiveness gaps that tend to limit the scope of the resulting partitioned methods to specific simulation scenarios. Data-driven system identification techniques provide an opportunity to close these gaps by enabling the construction of accurate, computationally efficient and minimally intrusive data transfer surrogates. This approach shifts the principal computational burden to an offline phase, leaving the application of the surrogate as the sole additional cost during the online simulation phase. In this paper we formulate and demonstrate such a surrogate-based partitioned method for a model advection-diffusion transmission problem by using Dynamic Mode Decomposition (DMD) to learn the dynamics of the interface flux from data. The accuracy of the resulting DMD flux surrogate is comparable to that of a dual Schur complement reconstruction, yet its application cost is significantly lower. Numerical results confirm the attractive properties of the new partitioned approach.

Deep and machine learning methodology in the context of application to computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CONFIGURABLE ML-POWERED DEFEATURING FOR SIMULATION

Steven Owen[*1]*

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ABSTRACT

In the rapidly evolving field of computational mechanics, the integration of machine learning (ML) has emerged as a transformative force. This abstract highlights our ongoing work at Sandia National Laboratories, where we leverage the power of ML to streamline and enhance the design-to-simulation process.

Design-to-simulation encompasses a multitude of intricate tasks, often characterized by their user-intensive, time-consuming, and error-prone nature. Our focus has been on identifying and targeting the most cumbersome aspects of this process, in collaboration with domain experts and analysts. Through close examination of their workflows, we endeavor to harness ML technologies to make their tasks more efficient, less prone to errors, and less tedious.

We have previously developed ML-based tools for defeaturing that employ a supervised learning procedure, utilizing decision tree methods. This approach, focused on enhancing design-to-simulation, has been a part of our ongoing efforts. This approach has proven to be both accurate and efficient. It not only predicts meshing outcomes but goes a step further by predicting the "best" CAD operations compatible with, Cubit(R), a CAD based tool used for geometry preparation and meshing.

The training of our ML models is grounded in a large dataset comprising thousands of CAD models and their corresponding meshes, along with the operations applied to them. This rich dataset forms the foundation upon which our ML algorithms make informed predictions, facilitating a smoother and more streamlined simulation process.

In this presentation, we will discuss our progress on a new configurable ML-based defeaturing environment. This environment incorporates the insights gained from our ML models, enhancing predictions for physics-specific simulation models. By combining the power of ML with the expertise of seasoned analysts, we aim to provide accurate predictions that not only optimize meshing but also select the most suitable CAD operations.

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Recent advances in numerical methods for interface problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MASS CONSERVATIVE FINITE ELEMENT METHOD FOR A NONISOTHERMAL NAVIER-STOKES/DARCY COUPLED SYSTEM

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ABSTRACT

We propose and analyze an H(div)-conforming and mass conservative finite element method for the coupling of nonisothermal fluid flow with nonisothermal porous media flow. The governing equations are the Navier-Stokes/heat system, commonly known as the Boussinesq system, in the free-fluid region, and the Darcy-heat coupled model in the membrane. These systems are coupled through buoyancy terms and a set of transmission conditions on the fluid-membrane interface, including mass conservation, balance of normal forces, the Beavers-Joseph-Saffman law, and continuity of heat flux and fluid temperature. We consider a velocity-pressure-temperature variational scheme for the Boussinesq system in the free-fluid region whereas in the membrane region we consider a dual-mixed formulation for the Darcy system coupled with a primal equation for the temperature model.
In this way, the unknowns of the resulting formulation are given by the velocity, pressure and temperature in both domains.
For the associated Galerkin scheme, we combine an H(div)-conforming scheme for the fluid variables and a conforming Galerkin discretization for the heat equation. Therefore, the resulting numerical scheme produces exactly divergence-free velocities and also allows preserve the law of conservation of mass at a discrete level. The analysis of the continuous and discrete problems is carried out by means of a fixed-point strategy under a sufficiently small data assumption. We derive optimal error estimates under an additional assumption over the data and present numerical results illustrating the performance of the method.

FIBREPLUG: A MULTISCALE TEXTILE COMPOSITES MODELING TOOL

Jide Oyebanji[1], Changze Sun[1], Mohamed Nasr Saleh[1], Kapil Krishnan[1] and Zhongwei Guan[1]*

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ABSTRACT

This study introduces a novel multi-scale modeling tool, FibrePlug [1], which advances the understanding of mechanical behavior of textile composites; combining the characteristic computational efficiency of macro-scale modeling with the ability to observe mechanical behavior of bundled filaments, which micro-scale modeling offers. When observed across multiple scales, the behavior of fibre reinforced polymer (FRP) composites significantly deviates as a function of the geometric scale under which such behaviors were observed [2]. This study, therefore, is particularly important as such understanding of the behavior of FRP across multiple scales becomes critical to the design and manufacture of components made from them. Previous attempts made towards the generation of meso-scale fabric models were limited to studying the material behavior at yarn level [3], leaving unresolved, the challenge of investigating filament-level response to practical loading applications including impact and stitching.

FibrePlug, the tool introduced in this research, is an open-source plug-in for multiscale modeling of textile composites. Developed within the ABAQUS Really Simple GUI (RSG) and Fox GUI development environments, FibrePlug advances the understanding of the behavior of composite materials beyond the limits imposed by traditional homogeneous macro- and meso-scale modeling. The plug-in allows for cross-scale modeling of textile composites.

The woven textile composite models generated with FibrePlug were validated experimentally by observing the mechanical deformation of bundled filaments under loading conditions imposed as a result of through-thickness stitching. This behavior and effective properties were observed with varying pin sizes and materials. This research opens a new domain of possibilities into investigating the responses of woven textile composites under different industrial applications including automobile, aviation and defense.

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A TWO-SCALE HIERARCHICAL PHFGMC FRAMEWORK FOR THERMO-MECHANICAL PROPERTIES OF C/C-SIC CMCS

Royi Padan[*1], Chen Dahan-Sharhabani[1], Omri Regev[2] and Rami Haj-Ali[1]*

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ABSTRACT

A state-of-the-art ceramic matrix composites (CMC) design for space or hypersonic applications requires a reliable and cost-effective method for predicting, estimating, and quantifying their mechanical properties. CMCs present complex anisotropic mechanical properties. Relating the properties to the specific CMC's composition and weaving architecture is expected. However, CMCs, especially C/C-SiC, are also highly affected by the microstructure of the local multi-phase material. Therefore, it is unsurprising that many recent studies employed different micromechanical models to evaluate CMCs' material properties.

Advanced micromechanical modeling of CMCs needs to balance computational demand and proper depiction of the local microstructure. The parametric high-fidelity generalized method of cells (PHFGMC) is an efficient numerical method to solve such detailed and relatively large-size computational problems [1]. Several works have already used the general method of cells to capture the elastic properties of a filament wound C/C-SiC [2] or even to evaluate the thermo-mechanical damage of a C/SiC CMC [3]. However, these studies have some limitations, such as using a linear displacement formulation (hence, ignoring the inter-phase tension shear coupling) and describing the complex structure using an idealized geometrical model.

The current study develops a two-scale hierarchical, PHFGMC-based framework to evaluate the thermo-mechanical properties of a C/C-SiC CMC. The repeated unit cells (RUC) are defined based on Computed tomography (CT). Both nano-CT (having a 1-micron resolution) and micro-CT (10-micron resolution) techniques were used to extract different geometrical models in a two-scale hierarchy. Finally, two PHFGMC micromechanical models are nested and integrated to represent the CMC micro and meso material levels. The proposed multiscale PHFGMC framework enables a realistic depiction of the material structure and allows for calculating the effective orthotropic properties of a single layer. Preliminary calculations show good agreement with test results. The proposed modeling can be used to design a broad class of CMC materials with different weave architectures and serve as a basis for damage evaluation prediction.

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Advances in multi-scale, multi-material, and multi-component Topology Optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VOROTO: MULTISCALE TOPOLOGY OPTIMIZATION OF VORONOI STRUCTURES USING SURROGATE NEURAL NETWORKS

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ABSTRACT

Cellular structures found in nature exhibit remarkable properties such as high strength, high energy absorption, excellent thermal/acoustic insulation, fluid transfusion, etc. Many of these structures are Voronoi-like; therefore researchers have proposed Voronoi multi-scale designs for a wide variety of engineering applications. However, designing such structures can be computationally prohibitive due to the multi-scale nature of the underlying analysis and optimization.
In this work, we propose the use of a neural network (NN) to carry out efficient topology optimization (TO) on multi-scale Voronoi structures. The NN is first trained using Voronoi parameters (cell site locations and associated thicknesses) to predict the homogenized constitutive properties. This network is then integrated into a conventional TO framework to minimize structural compliance subject to a volume constraint. Special considerations are given for ensuring positive definiteness of the constitutive matrix and maintaining microstructural connectivity. Several numerical examples are provided to showcase the proposed method.

IMPLEMENTING INTEGRATED EARTHQUAKE SIMULATOR FOR SEISMIC PERFORMANCE ASSESSMENT OF INDIAN CITIES

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[3]Earthquake Research Institute, The University of Tokyo

ABSTRACT

As per the records of National Center of Seismology of Indian government, more than 100 earthquakes of magnitude 3.0 or higher occurred in Indian sub-continent or neighboring region, which is evidence of increased frequency of seismic activities in the region. Increased frequency of seismic events has raised the concern over resilience of built environment in India. Moreover, unplanned Indian cities which are mainly comprised of un-engineered structures built in highly vulnerable land, are anticipated to put around 200 million city dwellers to risk against earthquake or earthquake induced disaster by 2050 according to reports of world bank and United Nation. Therefore, it is necessary to strengthen our built environment and seismic assessment is the first step in that direction.

In contrast to conventional study of seismic response of individual structures, performance analysis of cluster of structures is essential to assess the damage at city level so that officials and residents can choose reasonable preparation to mitigate the losses of earthquakes. Moreover, modeling of entire earthquake event i.e., generation and propagation of an earthquake, responses of structures and damage, and actions by people and communities for earthquake damage is required. To do this, a digital model of city is pre-requisite. More importantly, a numerically efficient tool is also needed.
Integrated Earthquake Simulation (IES) provides different predictions of earthquake hazards and disasters depending on the earthquake scenario. With the help of Geographical Information System (GIS), IES automatically construct the computer model of any city. IES perform the soil amplification analysis, seismic response analysis and mass agent simulation to mimic the entire event of earthquake.

We have used IES to simulate the three different earthquake events scenarios in the selected region of New Delhi. We obtained the total displacement and storey drift in each building against 1995 Kobe Earthquake, 2001 Bhuj Earthquake, and 2015 Gorkha Earthquake. In modeling the 2015, Gorkha Earthquake, a synthetic ground motion has been used, which is generated by combining three major seismic waves of earthquake. The preliminary results suggest that buildings which are five storey or higher have higher value of storey drift.

Geometric mechanics formulations and structure-preserving discretizations for continuum mechanics and kinetic models
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STRUCTURE PRESERVING DISCRETIZATION FOR THE LINEAR WAVE EQUATION

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ABSTRACT

Structure-preserving discretisations, by construction, enable the conservation of many invariants of the dynamics of PDEs. For example, energy, momentum, helicity (or enstrophy in 2D), in the Navier-Stokes equations, also potential enstrophy in the shallow waters equations, magnetic and cross helicity in MHD, etc. Besides the formal relevance, there are also concrete practical benefits of employing numerical discretisations that preserve some of the structure of the original equations. Structure preserving discretisations fundamentally rely on a set of function spaces that constitute a discrete de Rham sequence.

Most structure preserving discretization approaches address time evolution in a standard space plus time manner. Spatial finite-dimensional function spaces that constitute a de Rham sequence are employed for the spatial discretization and then a choice is made among the many available time integration methods.

There is a growing interest in numerical techniques for direct spacetime discretization (where time is address as any other coordinate). The potential advantages of this approach are, for example: spacetime anisotropic adaptivity, unified algorithmic parallelism, arbitrary order in spacetime.

In this work we will focus on the linear wave equation as a prototypical example for investigating different structure preserving time integration approaches. We will investigate a standard leap-frogging approach, ADER time stepping time integrator, and compare it to a spacetime structure preserving approach. We will discuss the spacetime de Rham complex and the spacetime formulation of the linear wave equation in differential geometry.

IMPLICIT NEURAL REPRESENTATIONS MEETS INTERPRETABLE PARAMETERIZED REDUCED-ORDER MODELING

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ABSTRACT

Learning interpretable reduced-order models of nonlinear PDE dynamics have been a long-standing problem in data-driven modeling of dynamical systems. Early works can be traced back to Operator Inference, Sparse identification of nonlinear dynamics (SINDy) and Sindy-Autoencoder, etc. However, these approaches still suffers from scalability issues of scalable nonlinear dimensionality reductions. On the other hand, novel dimensionality reduction framework that leverage implicit neural representation such as Neural Implicit Flow shows great promises on scalable 3D PDE data even on dynamic mesh. Here we propose a novel framework combining the idea of implicit neural with learning interpretable nonlinear dynamics from data. We compared our framework against state-of-the-art operator learning techniques (e.g., FNO) and a recent related work called DINo that leverages a vanilla feedforward neural network to learn the nonlinear latent dynamics. Furthermore, we extended our interpretable reduced-order learning framework to a parametric setting. Our testing cases range from wave equations, forced 2D Naiver Stokes equations to incompressible flow over a 2D cylinder.

Quantum scientific computing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

QUANTUM ANNEALING-BASED SOLUTION METHODS FOR TOPOLOGY OPTIMIZATION

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ABSTRACT

This talk presents quantum annealing-based solution methods for topology optimization (TO). Both convex and non-convex TO problems are considered. According to the problem's properties and structure, appropriate sub-problems are formulated so that they can be solved on an annealing-based quantum computer. In particular, the methodology can effectively tackle TO problems formulated as mixed-integer nonlinear programs (MINLP). Acknowledging the present limitations of quantum hardware, each MINLP problem is partitioned into two parts, so that the resulting sub-problems are adequately compact and hence solvable on currently accessible quantum computers characterized by a scarcity of qubits and limited connectivity. The first part can be efficiently solved on classical computers, while the second part with a reduced number of variables is solved on a quantum computer. By such, practical TO problem of varying scales can be handled on near-term quantum annealers. Computational efficiency and solution quality are assessed through solving a selection of benchmark TO problems and conducting comparisons with classical methods commonly employed in the field. This research offers pragmatic avenues for integrating quantum computing into the realm of TO, presenting the potential for leveraging quantum advantages in the practical design of topologies for diverse applications.

Machine learning methods for multiscale and multiphysics material modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MACHINE-LEARNING-BASED ASYMPTOTIC HOMOGENIZATION AND LOCALIZATION CONSIDERING BOUNDARY LAYER EFFECTS

Xiwei Pan[*1], Zhengcheng Zhou[1], Chuang Ma[1], Shaoshuai Li[1] and Yichao Zhu[1]*

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ABSTRACT

Asymptotic homogenization offers a way to efficiently analyze the mechanical behavior of multiscale configurations. But near a multiscale boundary, the homogenization strategy should be modified, as the underlying periodicity assumption breaks down there. In this article, we introduce a machine-learning-based asymptotic homogenization and localization scheme to formulate such boundary layer effects. To this end, we define a set of boundary layer cells, where external loading conditions are imposed on one side of the cell, and matching conditions with the interior periodic cells are imposed on the opposite side. The proposed theory identifies a mathematical expression for equivalent surface elasticity constants, surface balance equation and surface energy corresponding to periodic and spatially-varying microstructures due to the boundary layer presence. Implied from the asymptotic results, neural networks can be trained to memorize the interrelationship between key local quantities, such as the magnitude of the local maximum von Mises stress, and the local mechanical and geometric features, so as to avoid the repeated calling of cell problems when conducting failure estimation. Equipped with the trained neural networks, the online calculation for key (boundary-localized) quantities of interest under arbitrary loading conditions is expected to be accelerated substantially.

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Recent advances in high-order methods for computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HALF-CLOSED DISCONTINUOUS GALERKIN DISCRETISATIONS

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ABSTRACT

We introduce the use of half-closed nodesets where nodes in each element are placed only on a subset of element boundaries in Discontinuous Galerkin (DG) methods. This is as opposed to more commonly seen closed nodesets in DG, whereby in each element nodes are placed on all element boundaries. This provides extra freedom in the choice of node placement which we show allows for more efficient assembly of DG operators compared to closed nodesets. We also consider the effect of this choice of nodeset on commonly used linear solver techniques such as static condensation and block-based methods such as block-Jacobi, and outline some advantages to using half-closed nodes for these solver methods. Finally we demonstrate its use on a range of test problems including in CFD, and benchmark its performance on these numerical examples.

Computational and analytical advances in nonlocal modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ACCURATE ABSORBING BOUNDARY CONDITIONS FOR TWO-DIMENSIONAL PERIDYNAMICS

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ABSTRACT

The aim of this talk is to construct accurate absorbing boundary conditions (ABCs) for the two-dimensional peridynamics equation of motion which describes nonlocal phenomena arising in continuum mechanics based on integrodifferential equations. To this end, a full discretization of the system is used based on a Crank-Nicolson scheme in time and an asymptotically compatible scheme in space. Recursive relations for the Green's functions are then derived and numerically used to evaluate the nonlocal ABCs. In particular, these absorbing boundary conditions solve the corner reflection problem with high precision. The numerical analysis of the complete fully discretized scheme is implemented and numerical examples are finally reported to demonstrate the validity of the resulting ABCs.

Nanomechanics and nanoscale thermal transport for new materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ASSESSING THE IMPACT ON THE GLASS TRANSITION TEMPERATURE OF BITUMINOUS BINDER FROM ULTRA-THIN DIAMOND NANOTHREAD

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ABSTRACT

The nature of the glass state has been recognized by Science as one of the 125 challenges urgently awaiting resolution in the 21st century [1]. Despite decades of theoretical studies, the nature of the glass transition remains ambiguous and debated, while none has definitively addressed the issue [2]. We herein attempt to assess this complex phenomenon to events occurring at the molecular scale.

This work focuses on bitumen as the research subject, primarily comprising two parts. One aspect involves utilizing a data-driven model to accurately identify the glass transition region in molecular dynamics. By taking the derivative of the volume, we clearly captured the glass and rubber states. The other aspect involves introducing diamond nanothread (DNT) as a means to explore, from the perspective of molecular movement and microstructural arrangement, how the structure can regulate the glass transition temperature (Tg). DNT fillers induce inhomogeneity, which would promote the motion of small molecules while hindering the motion of large molecules□resulting in a higher Tg.

Glass transition region in this study is captured by simultaneously considering macroscopic volume and microscopic structure, which could move one step closer to unveil the mystery of the glass state, contributing to the broader comprehension of this intricate scientific challenge.

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COMPARING PARAMETER ESTIMATION OUTCOMES BETWEEN PHYSICS INFORMED NEURAL NETWORKS AND BAYESIAN METHODS

Michael Pantano[*1], Brandon Robinson[1], Jodi D. Edwards[2], Tetyana Kendzerska[3], Abhijit Sarkar[1] and Nastaran Dabiran[1]*

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[3]*Ottawa Hospital Research Institute*

ABSTRACT

The expanding field of machine learning has led to many branching approaches to data driven learning of mechanistic models. One of these branches is physics informed neural networks (PINN), which incorporates the use of a physics-based model to guide how the network learns [1]. Grounding the learning with a physical underpinning extends the standard neural network beyond a simple 'black box' model and provides a mechanism to perform parameter estimation of the imposed mechanistic model. Parameter estimation within a typical PINN involves frequentist statistics. In this talk, we compare its suitability as a method for parameter estimation to standard approaches in inverse modelling using Bayesian inference [2].

We present a series of numerical investigations considering various PINN architectures, assessing their capacity to estimate system parameters and compare their outcomes to benchmark results obtained using Bayesian inference under similar conditions. The first architecture type considered is the more common representation of a PINN, which embeds physics into the loss function [1]. The second architecture type tested embeds the assumed physics into the units of the neural network itself [3]. We compare and contrast these methodologies for two dynamical systems governed by ordinary differential equations. Specifically, from engineering mechanics, we consider the vibrations of a mass-spring system, and from infectious disease modelling, we consider population-level disease transmission using compartmental models.

This talk aims to assess the strengths and weaknesses of PINNs against established methods for Bayesian inference for the task of parameter estimation and subsequently for forecasting. The objective is to better understand of these two different paradigms, and additionally to compare the performance of different PINN implementations.

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A CONSISTENTLY LINEARIZED STOCHASTIC FINITE ELEMENT FORMULATION FOR GEOMETRIC NONLINEAR COMPOSITE SHALLOW SHELLS

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ABSTRACT

Material properties such as young's modulus are subject to uncertainties. This natural variability is called aleatory uncertainty and cannot be reduced. The influence of uncer tain structural parameters on the behavior of mechanical structures is considered in the context of stochastic structural analysis. Due to the stochastic modeling of material properties, the quantities of interest, e.g. displacements and stresses, are random variables. The Monte Carlo Simulation (MCS) is a widely used method to estimate statistics such as mean value, variance and higher moments of these variables. Although the MCS is very flexible, it is impractical with respect to computational time. The polynomial chaos expansion (PCE) is a particularly efficient way to replace the necessary computationally expensive MCS [1]. Within the spectral stochastic FEM (SSFEM), the PCE is directly integrated into the FE formulation of structural elements [2]. The application of the SSFEM to geometric nonlinear mechanical structures remains comparatively unexplored. In this contribution, the SSFEM is applied to geometric nonlinear shell structures of composite material under the influence of uncertain structural parameters such as material and geometrical properties. A comparison of results of the SSFEM and the MCS shows the efficiency of the method. Special focus is set on the consistent linearization, which is necessary to achieve quadratic convergence in the context of a Newton iteration scheme. Furthermore, the polynomial degree is investigated, which has a strong influence on the quality of the results. Challenging tasks such as limit points in stability analysis are examined, which includes studies on the convergence behavior of the extended FE formulation. In addition, the sensitivity of the uncertain input parameters to the quantity of interest are part of the investigations.

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Computational mechanics for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELLING OF SOLUTE TRAPPING AND NON-EQUILIBRIUM MICROSTRUCTURE DURING RAPID SOLIDIFICATION OF ADDITIVE MANUFACTURING

Chinnapat Panwisawas[*1]*

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ABSTRACT

Understanding the underlying mechanisms of metal additive manufacturing (AM) through computational materials engineering necessitates to materials design and process optimisation. The stochastic nature of emerging AM microstructure induced by thermal-chemical-fluid dynamics is the key to maximise the AM performance. It is likely induced by metal powder size/shape distribution, energy input by process parameters, processing-induced defects (e.g. porosity, crack), and second phase precipitation, which all result in heterogeneous non-equilibrium microstructural variations and site-specific behaviour. Solute element transport during rapid and repeated thermal cycle in metal AM which is able to induce non-equilibrium, non-uniform microstructure remains unprecedented. We have developed a computational materials engineering approach to reveal the solute transport induced by melt convection which dilutes the partitioned solute at the solidification front and promotes solute trapping and elucidates the mechanisms of the subsequent microstructural transitions to ultra-fine cells and then to coarse cells. These suggest solute trapping effect could be made used of for reducing crack susceptibility by accelerating the solidification process. The detailed solidification pathway exhibits promising potential for additively manufactured ‘hard-to-print’ superalloys and aids the future materials design for better 3D printability.

Advanced machine learning methods for multiscale modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A COMPACT QUANTUM MACHINE LEARNING FRAMEWORK PREDICTING PROPERTIES OF COMPLEX MATERIALS

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[1]Academia Sinica

ABSTRACT

Machine learning (ML) is increasingly being leveraged to predict complex material properties, such as potential energies. Traditional ML models are parameter-dense, often containing thousands to hundreds of thousands of parameters, and typically estimate global properties based on localized atomic contributions —neglecting long-range interactions. We introduce a quantum machine learning (QML) framework designed to overcome these limitations by accurately predicting energies of complex material systems. This framework employs a renormalization technique that condenses atomic descriptors into a feature map, facilitating the encoding of systems with any atom count into a quantum ML circuit utilizing fewer than ten qubits. Utilizing two novel QML circuit architectures, the quantum convolutional neural network (QCNN) and the quantum deep neural network (QDNN), our models, with fewer than one hundred parameters, achieve significant predictive accuracy for both Co0.25Ni0.25(HfTiZr)0.5 complex alloy and lead-based metal-organic frameworks (MOFs). This ultra-compact QML approach, with parameter counts drastically lower than those in classical models, offers a scalable solution for predicting the energetics of complex materials of varying sizes.

Computational modeling of extreme-loading events
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ALASKA WALL SYSTEM: EXPERIMENTAL AND NUMERICAL COMPARISONS OF A COST-EFFECTIVE MITIGATION SCHEME

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ABSTRACT

Under the auspice of the international cooperation SHIELD, a specific test wall arrangement was tested at Ft. Polk, Louisiana, USA, in 2021.

The idea behind this exercise was to emulate a “planter-type” structure which can be used as a mitigation scheme both in urban environments and the military theater. This specific arrangement consisted of two (2) rows of three (3) Alaska wall units that were buried 1.45 m below the surface, thus exposing 2.25 m of clear wall aboveground. The two sets of walls were separated by 2.0 m (clear distance). The in-between void was filled with indigenous material (a combination of sand and silty clay type of soil). The overall arrangement was subjected to a close-in detonation at a scaled distance of 0.4 m/kg(1/3), in TNT equivalent terms.

This presentation discusses the establishing of the loading environment (CFD analyses), the generation of a series of Lagrangian FE models (CSM analyses) in predicting the structural response, and comparison of experimental and numerical results. Shortcomings and difficulties encountered during this project will also be discussed.

Modeling and simulation of advanced manufacturing processes for metals
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

QUANTITATIVE BENCHMARK FOR LASER POWDER BED FUSION MELT POOL SCALE MODELS

Hélène Papillon-Laroche[1], Amishga Alphonius[1], Magdalena Schreter-Fleischhacker[2], Yohann Vautrin[3], Florin Ilinca[4], Jean-Philippe Harvey[1] and Bruno Blais[1]*

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[3]*National Research Council Canada*
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ABSTRACT

Laser Powder Bed Fusion (LPBF) is a 3D printing process using metal powder as the raw material. A laser selectively melts the powder bed, and the raw material is consolidated using a layer-by-layer building strategy. At the melt pool scale, solid-liquid phase change, surface tension and evaporation effects are involved, and their highly dynamic interaction drives the melt pool (MP) morphology, thermal history, and the occurrence of defects in the final part. To predict the latter, high fidelity thermo-fluid models are currently used. However, precise knowledge and quantification of the model errors and their sources is absent as verification and validation are either disregarded or incomplete. This hinders meaningful insight from the current LPBF MP predictions.

This work proposes a reproducible quantitative benchmark to evaluate the accuracy and adequacy of LPBF MP scale models. It is twofold: verification via a code-to-code comparison and validation with experimental data. It focuses on the static irradiation of a bare plate of Ti-6Al-4V, experimentally studied by Cunningham et al. [1]

The code-to-code comparison of results is performed using selected high-fidelity thermo-fluid models. Space and time refinement studies are proposed to analyze the sensitivity of the solution to the chosen discretization. Targeted verification metrics are the MP and vapor depression (VD) dimensions, and temperature gradients. Monitoring of the error norms assesses if the different thermo-fluid models converge to the same reference solution, defined as the solution obtained with the finest discretization. The second part of the benchmark assesses the models' adequacy using Cunningham et al. [1] experimental results. This validation step focuses on the temporal evolution of the MP and VD dimensions, and we are interested in the predictive capacity of the models for the different melting modes encountered in the experimental setup.

The presentation focuses on the benchmarking of two diffuse finite-element based thermo-fluid frameworks, developed by independent groups: Lethe from Polytechnique Montréal, and MeltPoolDG from the Technical University of Munich. It also aims to advertise this new benchmark to other research groups and encourage them to verify and validate their thermo-fluid models using the proposed studies. Hence, it provides the required numerical results to compare their own solutions. Special care is taken to thoroughly describe the benchmark case, material properties, and solver parameters ensuring reproducibility.

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speed x-ray imaging," Science, vol. 363, no. 6429, pp. 849–852, Feb. 2019. https://www.science.org/doi/10.1126/science.aav4687

Physics-based data-driven modeling and uncertainty quantification in computational materials science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GOAL-ORIENTED CALIBRATION OF MODELS AND ASSOCIATED MODELING ERRORS

Antonin Paquette-Rufiange[*1], Serge Prudhomme[1] and Marc Laforest[1]*

[1]*Polytechnique Montréal*

ABSTRACT

Models of increasing complexity are now commonly used to predict quantities of interest for physical systems at various scenarios. However complex these models are, they are but abstractions of the system of interest. They involve simplifying hypotheses, which induce some modeling errors; in other words, they only provide approximate responses of the system of interest. Such hypotheses usually introduce unknown parameters, the so-called model parameters, that need to be calibrated. The formulation of the calibration process will directly affect the values of the calibrated parameters, the modeling error in the model, and hence the predictive capability of the model.

We propose a novel approach for calibration that identifies both the model parameters and the modeling errors. Our calibration process relies on the fact that each value of the model parameters generates its own model with associated modeling errors. For a given value of the model parameters, we calibrate the modeling error by representing it as a Gaussian process, as proposed by Kennedy and O'Hagan [1]. More precisely, we calibrate the (hyper)parameters of the modeling errors via maximum likelihood [2]. The novelty of our calibration approach resides on how the values of the model parameters are inferred, that is, we define an objective functional with respect to the intended use of the model and seek the model parameters that minimize a functional of the modeling errors. For example, one goal may be to minimize the modeling error at a specific scenario or for a set of scenarios of interest. The proposed approach is therefore referred to as a goal-oriented method for calibration of the model parameters.

The pertinence of this approach will be illustrated on a simple problem to highlight the influence of the modeling errors on the calibration of the model parameters. This example will also illustrate that our methodology alleviates the identifiability problem between the modeling errors and the model parameters. The calibration process will further be applied to the thermal problem presented at the Sandia Challenge 2008. Different objective functionals will be studied, demonstrating the versatility of our approach and the way it can improve the predictive capability of a model.

[1] M. C. Kennedy and A. O'Hagan. Bayesian calibration of computer models. Journal of the Royal Statistical Society: Series B (Statistical Methodology), 2001

[2] N. Leoni, O. Le Maître, M.-G. Rodio, and P. M. Congedo. Bayesian calibration with adaptive model discrepancy. International Journal for Uncertainty Quantification, 2024

UQ-TTA student paper competition in uncertainty quantification
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GOAL-ORIENTED CALIBRATION OF MODELS AND ASSOCIATED MODELING ERRORS

Antonin Paquette-Rufiange[*1], Serge Prudhomme[1] and Marc LeForest[2]*

[1]Polytechnique Montréal
[2]Polytechnique Montréal)

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Models of increasing complexity are now commonly used to predict quantities of interest for physical systems at various scenarios. However complex these models are, they are but abstractions of the system of interest. They involve simplifying hypotheses, which induce some modeling errors; in other words, they only provide approximate responses of the system of interest. Such hypotheses usually introduce unknown parameters, the so-called model parameters, that need to be calibrated. The formulation of the calibration process will directly affect the values of the calibrated parameters, the modeling error in the model, and hence the predictive capability of the model.

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[2] N. Leoni, O. Le Maître, M.-G. Rodio, and P. M. Congedo. Bayesian calibration with adaptive model discrepancy. International Journal for Uncertainty Quantification, 2024

Numerical modelling of composite materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL ANALYSIS OF POST-TENSIONED WALLS' MECHANICAL BEHAVIOR FOR HOUSING VIA A SIMPLIFIED MODEL OF ITS CONSTITUTIVE TENSOR

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ABSTRACT

Housing construction requires industrialized and efficient construction procedures that allow the massive construction of housing, providing the required quality of life. The post-tensioned concrete system has been adapted to develop post-tensioned walls that allow the prefabrication of homes and their assembly in the field. The experimental tests applied to this type of wall, built at full scale, establish the structural parameters and their performance capacity under static load.
Previously, constitutive models have been proposed based on an isotropic damage model for concrete modeling, the classical elasto-plasticity theory for bar modeling, and the elasticity theory for post-tensioning cables. Combining the three models through mixing theory reflects their mechanical behavior for implementation in numerical simulation. The complexity of the interaction of the models lends itself to using code developed expressly for this type of simulation.
This document establishes a methodology for the simulation of post-tensioned concrete walls through commercial programs using a simplified model for their characterization and analysis, whose input will be the constitutive tensor of the composite material assigned to each finite element. The constitutive matrix of the composite material will be computed considering the percentages of volumetric participation of the simple materials that compose it, the working orientation of the fiber-type materials through the theory of series/parallel mixtures, and the inclusion of the axial deformation of the cable as an effect of post-tensioning.

Keywords: Post-tensioned concrete, Series/Parallel Mixing Theory, Numerical Simulation, Imposed Unitary Strain

Advances in computational mechanics for flow-induced vibrations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A GRAPH NEURAL NETWORK BASED REDUCED-ORDER MODEL FOR FLAPPING DYNAMICS

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ABSTRACT

An elastic foil, cantilevered at the trailing edge, also known as the inverted foil, exhibits an intriguing self-induced flapping motion when exposed to fluid flow. This fluid-structure interaction phenomenon holds significant interest for its applications in renewable energy harvesting. In this study, we numerically investigate how inverted foil's response changes when positioned in tandem with a stationary circular cylinder. The problem is modeled using a higher-order variational solver, incorporating fully coupled three-dimensional Navier-Stokes and nonlinear structural equations. This methodology is based on the combined field explicit interface formulation proposed by [1]. Our observations reveal that for a specific range of parameters, the flapping motion is wake-induced, driven by synchronization between the foil's motion and the shedding of vortices from the cylinder. Consequently, the foil demonstrates sustained and controlled oscillations, rendering it ideal for efficient energy harvesting. To further enhance energy efficiency and fortify the design of resilient energy harvesting systems, parameter optimization becomes crucial.

Effective optimization using traditional computational simulations involves performing analysis over a wide parameter spectrum which is both time-consuming and computationally expensive. Addressing this challenge, we propose a graph neural-based reduced-order model (GNN-ROM) tailored specifically for the inverted foil problem. This model adeptly handles mesh-structured data involved in full-order simulations without necessitating modifications, allowing it to effectively simulate fluid-structure interactions efficiently and faster. Our model uses the rotation equivariant, quasi-monolithic GNN proposed by [2]. This framework is based on the arbitrary Lagrangian-Eulerian formulation, wherein time series prediction of the system states is made with two sub-networks. Essential coefficients describing mesh motion are extracted by proper orthogonal decomposition, which are predicted over time using a single multilayer perceptron. Simultaneously, the GNN-ROM evolves the flow field based on the system state. The structural state is implicitly modeled by the mesh movement on the solid-fluid interface. This proposed model is currently undergoing training and validation using our full-order simulation data. Once established, it stands poised to serve as a robust surrogate model for the inverted foil, facilitating the fast parametric optimization and control of inverted foil-based energy harvesting devices.

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Scientific machine learning for geophysical applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SYNTHETIC INFLOW TURBULENCE GENERATION BASED ON CONDITIONAL NEURAL FIELD ENCODED LATENT DIFFUSION MODEL

Meet Hemant Parikh[*1], Xin-Yang Liu[1], Pan Du[1], Xiantao Fan[1] and Jianxun Wang[1]*

[1]*University of Notre Dame*

ABSTRACT

Eddy-resolving turbulence simulation techniques, such as Direct Numerical Simulations (DNS) and Large Eddy Simulations (LES), often necessitate the generation of stochastic inflow boundary conditions. Conventionally, people employ recycling-based approaches, which involve conducting a separate, fully turbulent flow simulation under periodic boundary conditions. The turbulence field obtained from this precursor simulation, upon reaching a statistically steady state, is then utilized as the inlet condition for the primary simulation. Although this approach effectively captures the statistical and dynamical properties of turbulence, it is computationally demanding and time-intensive. Alternatively, various synthetic inflow turbulence generators have been developed, including methods like the synthetic random Fourier method, synthetic digital filtering method, and synthetic coherent eddy method, among others. These synthetic techniques are designed to efficiently synthesize inflow turbulence on-the-fly without the need for extensive precursor simulations or data storage requirements. However, they often struggle to accurately replicate the complex dynamical properties and coherent structures of true turbulence. This shortfall frequently results in considerable computational overhead, due to the need for a larger computational domain to dissipate nonphysical features and allow for the re-development of turbulence within the primary simulations.

Recent developments in deep learning have offered new solutions for turbulent inlet generation. Existing explorations have utilized sequence models like Long Short-Term Memory (LSTM) and transformers to learn the dynamics from simulation data. However, these models often encounter error accumulation during long-term rollout predictions, especially for chaotic and turbulent regimes. Additionally, their ability to handle the stochastic nature of turbulence is limited. Although generative models, such as Generative Adversarial Networks (GAN), show promise, they are challenging to train and often lack generalizability across different flow conditions or meshes. To address these issues, we propose a method leveraging both conditional neural fields (CNF) and latent diffusion models (LDM). This technique uses CNF to encode spatiotemporal features into a hidden space, where LDMs generate new samples based on varying Reynolds numbers. By harnessing the strengths of both CNF and LDM, we are able to build an effective, mesh-independent inlet turbulence generator for various flow conditions.

Modeling and simulation of coupled processes in geological media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ON THE VIABILITY OF SALT CAVERNS FOR MASSIVE STORAGE OF HYDROGEN BY USING NUMERICAL SIMULATION

Jose Paris[*1], Andrés Soage[12], Blanca Fernández[1], Francisco Figueiras[1], Ignasi Colominas[1] and Luis Cueto-Felgueroso[2]*

[1]*University of A Coruña*
[2]*Polytechnic University of Madrid*

ABSTRACT

Massive storage of energy has been a challenge for society and an cheap, secure and reliable solution has not been achieved. Hydrogen seems to play a crucial role in the future energetic mix but among many other considerations it requires very large storage volumes to face the energetic demand nowadays. Underground salt caverns are being considered as an efficient and cheap alternative for hydrogen storage at industrial scale. This research is devoted to analyze by numerical simulation the conditions, viability and efficiency of using salt caverns. The developed models involve non linear structural analysis, creep, fatigue, thermal effects, dynamic simulations and many other relevant aspects [1].

Stability and viability conditions must be determined both in dome formations and in bedded saline ones since they equally appear in nature. The models developed consider the effects of geothermal gradient with the depth and its effect on nonlinear structural phenomena and non linear halite formations. Furthermore, operating conditions and different operation cycle configurations by means of maximum and cushion gas pressures, and injection and withdrawal cycles among others are also analyzed to verify the most adequate strategy and the useful life of the facility under different operation scenarios. Maximum deformations allowed on the top of the cavern have demonstrated to be critical aspects for the viability of this type of geological storage systems and an expected useful life of 30 years is the goal. Taking into account these considerations our findings show that under adequate conditions, geometries and operating conditions salt caverns are an adequate option to store massive amounts of hydrogen and, consequently, of energy.

Finally, some application examples of applications under real conditions have been analyzed.

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MULTISCALE COMPUTATIONAL HOMOGENIZATION FOR FLOW THROUGH POROUS MEDIA

Thomas Paris[1], Vincent Bruyere*[2], Patrick Namy[2], Sylvain Chupin[1] and Denis Rochais[1]*

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ABSTRACT

Macroscopic modeling of flow through porous media requires knowledge of equivalent properties (permeability, conductivity, diffusivity) for calculations. Depending on microstructure topology and fluid flow regimes at the microscopic scale, great disparities in equivalent properties can be found in the literature.

Multiscale computational homogenization (EF^2) is shown to be an interesting tool and could be used as a guideline to choose with greater confidence the most suited formulation for specific porous media. A numerical twin strategy is used to surpass experimental limitations in order to describe flow through specific and complex porous microstructures. Analytical formulations for permeability at the macroscale are discussed and compared to lower scale calculations.

Finally, numerical twin strategy seems not only able to recover consistent permeability values but also to capture different mechanisms both sides of the spectrum such as inertia effect for high Reynolds number and wall effect for high Knudsen number and rarefied gas regime.

A REDUCED-BASIS METHOD FOR UNCERTAINTY QUANTIFICATION IN RANS SIMULATIONS OF HYPERSONIC TURBULENT FLOWS

Eric Parish[*1], Elizabeth Krath[1] and Patrick Blonigan[1]*

[1]*Sandia National Laboratories*

ABSTRACT

The Reynolds-averaged Navier—Stokes (RANS) equations are the workhorse analysis tool for simulating hypersonic turbulent flows in complex environments. Unfortunately, RANS models have uncertainties which can bias their predictions. This work presents a reduced-basis method (RBM) for quantifying parametric uncertainties in the RANS equations. Our approach leverages entropy variable transforms, a globalized Newton solver, and a quasi-multigrid solution strategy to construct a robust, stable, and accurate Galerkin RBM. We further equip this RBM with QoI-based error indicators to aid in greedy training and a posteriori error estimation. We present results on a suite of hypersonic flow problems, including the HIFiRE-1 ground test, and demonstrate the efficacy of our approach for UQ analyses.

Recent advances in numerical methods for interface problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

POLYGONAL STAGGERED DISCONTINUOUS GALERKIN METHODS FOR PROBLEMS IN POROUS MEDIA

Eun-Jae Park[*1]*

[1]*Yonsei University*

ABSTRACT

In this talk, we first present the staggered DG method on general meshes for the Poisson equation. Then, some applications to interface problems are considered such as coupling of Darcy-Forchheimer and Stokes equations, and a single-phase flow in porous media with a fracture. In the case of s fractured porous media, the bulk variables are solved using staggered DG method and an interface variable is solved using the continuous Galerkin method. We derive optimal convergence for both pressure and velocity fields. Numerical experiments suggest that our method is more accurate when polygonal meshes are used among various mesh configurations; moreover, our method is robust to mesh distortion. These observations allow us to consider unfitted methods without any special treatment. With background meshes generated independent of fracture, numerical solutions converge in optimal order.

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2. L Zhao, E. Chung, E-J Park, and G. Zhou, Staggered DG method for coupling of the Stokes and Darcy-Forchheimer problems, SIAM J. Numer. Anal. 59 (1), 1--31, (2021).

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Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL MODELING OF HYDROGEN EMBRITTLEMENT-INDUCED DUCTILE FRACTURE WITH GURSON-COHESIVE MODEL (GCM)

Jihyuk Park[1], Huh Nam-Su[2] and Kyoungsoo Park[1]*

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ABSTRACT

Hydrogen embrittlement fracture is essential in various industrial applications, particularly in ensuring the structural integrity, especially when a material is exposed to hydrogen-rich environments. Hydrogen embrittlement involves the diffusion of atomic hydrogen into the material lattice, interacting with various microstructural features. For instance, hydrogen enhanced localized plasticity (HELP) appears as hydrogen-enhanced plastic deformation localized around stress concentrators leading to microcrack initiation, while hydrogen enhanced decohesion (HEDE) mechanism involves the accumulation of hydrogen atoms at material interfaces inducing decohesion between grains or phases. In this study, a computational framework is presented, which integrates a ductile fracture modeling and a hydrogen diffusion modeling, to investigate the role of hydrogen in triggering localized plasticity and its subsequent impact on fracture initiation. For a ductile fracture modeling, the Gurson-Cohesive model (GCM) is employed. In GCM, the Gurson model represents continuum damage evolution while a finite element-based cohesive zone model describes crack surface discontinuity in conjunction with the traction-separation relation. The transition from continuum damage to discontinuous crack is defined using a crack initiation criterion, which accounts for porosity and triaxiality. The investigation extends to understanding the influence of hydrogen on the softening behavior of the traction-separation relationship on the discontinuous crack surface. Parametric studies explore the sensitivity of material properties and environmental conditions. This exploration describes the factors influencing fracture behavior from HELP and HEDE mechanisms, contributing to the identification of critical parameters for material susceptibility to hydrogen-induced fracture. By combining numerical models of hydrogen diffusion considering the HELP and HEDE mechanisms and the ductile fracture model, this study provides an understanding of hydrogen-induced fracture, contributing significantly to the ongoing efforts in designing materials resilient to hydrogen embrittlement in practical engineering applications.

Model order reduction for parametrized continuum mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THERMODYNAMICS-INFORMED LATENT SPACE DYNAMICS IDENTIFICATION (TLASDI) FOR REDUCED-ORDER MODELING OF DYNAMICAL SYSTEMS

Jun Sur Park[*1], Siu Wun Cheung[2], Youngsoo Choi[2] and Yeonjong Shin[3]*

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[3]*North Carolina State University*

ABSTRACT

In this work, we present a thermodynamics-informed latent space dynamics identification (tLaSDI) method for learning an intrinsic invariant manifold which comply with the first and second principles of thermodynamics from data. Our approach utilizes an autoencoder to provide a nonlinear latent representation and the reconstruction of the high-dimensional data, and the corresponding latent space dynamics are captured using GENERIC formalism informed neural networks (GFINNs). The GFINNs are designed to exactly satisfy the degeneracy condition of the GENERIC formalism, ensuring that the latent space dynamics adhere to fundamental thermodynamics principles, such as energy conservation and entropy inequality restrictions. To enhance the accuracy and efficiency of data-driven reduced-order modeling, we perform simultaneous training of the autoencoder and GFINNs. Additionally, we introduce the loss components based on rigorous error estimates to further improve the accuracy of the prediction. The numerical results demonstrate that the tLaSDI method shows great potential for enhancing the computational efficiency of high-dimensional dynamical systems while maintaining accurate predictions.

Trustworthy multi-fidelity and data-driven models for computational applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NEW MULTI-FIDELITY METHOD FOR HIGH-DIMENSIONAL PROBLEMS WITH DIFFERENT SETS OF INPUT VARIABLES

Youngseo Park[1] and Ikjin Lee*[1]

[1]*KAIST*

ABSTRACT

Many researches regarding multi-fidelity (MF) modelling have been studied in decades, due to its ability to construct accurate model despite of the limited number of high-fidelity (HF) data by utilizing a number of low-fidelity (LF) data. However, conventional MF methods construct a single model for the entire input space, which make them require numerous samples for high-dimensional problems having more than ten input variables. To alleviate this problem, MF methods combined with the high-dimensional modelling techniques, such as high dimensional model representation [1] and mapping [2], are proposed. Nevertheless, these methods assume that the input sets of MF data are consistent, which would not be true especially for high-dimensional problems. To solve this issue, new MF method is proposed for high-dimensional problem with different sets of input variables.

The proposed method categorizes input variables into three groups; common variables that are present in both LF and HF, variables that exist only in LF model, and those that exist only in HF model. First of all, LF model is built by using high-dimensional modelling technique. Subsequently, HF data are utilized to train the MF model by reflecting correlation of LF and HF responses. In the training process, the relationships of input variables only in HF and those only in LF are also trained, which make it possible to predict response of different input sets. Numerical examples show the proposed method construct accurate MF model in the high-dimensional problems having different input sets.

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Virtual elements for partial differential equations on polytopal meshes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ON TRIANGULAR SELF-STABILIZED VIRTUAL ELEMENTS FOR KIRCHHOFF-LOVE SHELLS

Tiago Park Wu[*1], Paulo de Mattos Pimenta*[1] *and Peter Wriggers*[2]

[1]*University of São Paulo*
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ABSTRACT

We present low-order triangular virtual elements for linear Kirchhoff-Love shells. The domain decomposition by flat triangles directly approximates the shell geometry without resorting to a curvilinear coordinate system or an initial mapping approach. In light of the available low-order virtual element procedures for each plane elasticity and plate bending problem, the membrane and plate are conveniently superposed in space. The serendipity VEM is applied for the membrane and we explore the stabilization-free VEM for the plate as an attempt to provide a starting point for its future evolution. A nonconforming plate scheme is withal considered. Numerical examples of static problems are presented to show the potential of our formulation to further Kirchhoff-Love shell virtual element developments.

Deep and machine learning methodology in the context of application to computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ON DEFINING A FEATURE AND LABEL SPACE FOR ML GUIDED DEFEATURING

Sam Parry[1] and Steven Owen*[1]

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ABSTRACT

In Computer-Aided Design (CAD), defeaturing is the process of optimizing 3D models for finite element simulation by simplifying or removing non-essential geometric features. Unnecessary complexity in the CAD part leads to overly complex meshes that require more resources to simulate. Despite the significance of defeaturing, the process remains a tedious, time-consuming task that relies on the expertise and in-situ decision making of a skilled analyst. Our research seeks to bridge the gap to automation by leveraging machine learning techniques to expedite defeaturing operations, reducing the manual workload on analysts and enhancing the efficiency of CAD model optimization. We propose a Machine Learning (ML) driven approach to defeaturing by which an analyst is shown a ranked list of operations ordered by their predicted improvement to mesh quality. We also propose a definition of a comprehensive feature and label space that can be used to train ML models for predicting the likely success and resulting mesh quality improvement of each possible defeaturing operation.
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Immersed-boundary variational methods: Theory, data structures, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DISCONTINUOUS FINITE CELL METHOD FOR PROBLEMS IN SOLID MECHANICS

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ABSTRACT

The finite cell method (FCM) starts with a regular mesh on a simple domain which embeds the domain of a PDE, and benefits from an arbitrary extension of the high-order approximation of the unknowns into the enveloping domain by assuming a very soft material in the extended region [1]. The method has been successfully investigated in a variety of problems in solid mechanics and beyond. The discontinuous finite cell method (DFCM) is not an extra step in FCM, but rather a natural step back to the phase before cell matrices are being assembled; thus solving the element equations of each cell almost independently, with the additional boundary conditions that arise from neighbouring cells. The main drawback, at first glance, is in increasing the number of degrees of freedom; however, this provides many opportunities to benefit from the advantages of both FCM and the discontinuous Galerkin FEM. While the FCM provides fast and simple solutions in dealing with inclusions as well with cells cut by the boundary, the discontinuous feature offers a good remedy for cells that are completely divided by material discontinuities, and makes it easy to add or remove cells, and thus to move boundaries.
In this paper, we present the formulation of the DFCM, and demonstrate its merits compared to similar methods using several examples.

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Mathematics and algorithms for predictive digital twins (DT)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BAYESIAN INFERENCE FOR PATIENT-SPECIFIC DIGITAL TWINS IN ONCOLOGY

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ABSTRACT

Uncertainty quantification is an essential component of a digital twin and plays a central role in establishing trust in the model's predictions and enabling robust decision making. This is particularly salient when digital twins are employed as enablers for personalized medicine [1,2]. While digital twins can play a key role in tailoring therapeutic interventions, the underlying mathematical and computational models must be calibrated with noisy data that are infrequently collected and may only be indirectly informative. In particular, mechanistic modeling of high grade gliomas proves challenging due to significant heterogeneity, both in physiology and response to treatment. This heterogeneity has also proved challenging in the clinic, resulting in low median survival rates despite an aggressive standard-of-care. We present a methodology that utilizes non-invasive quantitative magnetic resonance imaging (MRI) collected longitudinally. The first (post-operative) MRI sequence in the time course is used to generate a patient-specific computational geometry and assign initial conditions. Tumor extent and cellular density are estimated from the acquired MRI data and projected onto the computational domain. These data are then used to inform spatially varying model parameters in a reaction-diffusion partial differential equation (PDE) describing tumor invasion and proliferation through the solution of a Bayesian inverse problem. Specifically, we seek to compute the Laplace approximation to the posterior by first solving a PDE-constrained optimization problem to compute the maximum a posteriori (MAP) point. The inverse of the Hessian at the MAP point which is taken to be the covariance operator of a Gaussian centered at the MAP point. We comment on the ill-posed nature of the problem and the role that regularization plays in obtaining faithful reconstructions, highlighting how total-variation based regularization can capture sharp variations in the sought-after diffusion and proliferation rates that are associated with the underlying material interfaces of the anatomy (e.g. gray/white matter).

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Modeling and inverse design of architected materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELLING SYMMETRY BREAKING AND GEOMETRIC FRUSTRATION IN BISTABLE KIRIGAMI FOR ON-TARGET ANISOTROPIC MORPHING

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ABSTRACT

Programming the bistable morphing of kirigami metamaterials for flat-to-3D deployment is a challenging task due to the complexity of the slit pattern and the underlying physical relations between slit symmetry and geometric frustration. In this work I will present a material modelling strategy to generate anisotropic shape morphing in bistable kirigami that leverages symmetry breaking to induce geometric frustration in their deployed state. While current bistable kirigami deploys with preserving shapes that are frustration-free, here the entire morphing space is mapped to access anisotropic deployment yielding non-uniformly scaled shapes that are geometrically frustrated in their second state of equilibrium. I will explain the physical mechanism underpinning anisotropic deployment and elucidate the interplay between anisotropy, bistability, and scaling transformation. Finally, I will show examples of inversely designed kirigami where anisotropic deformation is leveraged to achieve target three dimensional shapes and functionalities so far unattainable with existing isotropically scalable kirigami.

Data-driven device and circuits models
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HAMMERSTEIN-WIENER DATA-DRIVEN COMPACT CIRCUIT MODELING. PART 1: MODEL FORMULATION AND TIME DOMAIN TRAINING.

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ABSTRACT

Circuit simulations, often referred to as Spice simulations, are foundational to modern circuit design, assessment and qualification. Traditional Spice simulations use circuit descriptions built from compact device-level models by applying Kirchoff's current and voltage laws. This leads to systems of differential algebraic equations (DAEs) that must be solved numerically. Unfortunately, this approach does not scale well across system hierarchy levels because the size of the underlying DAE is proportional to the number of discrete devices in the circuit. At the same time, many commonly used circuits (e.g., operational amplifiers, comparators, voltage regulators, etc.) have relatively simple scripted behaviors that can be captured by simpler models reproducing the relevant input-output relationships. Such behavioral circuit models are an alternative to detailed transistor-level simulations that can potentially address the simulations' scalability challenge at higher levels of system integration.

This talk is the first in a series of two talks where we present recent work to establish a data-driven framework for the rapid development and deployment of scalable behavioral models for functional circuit blocks. To that end we consider circuit models having canonical system identification architectures, such as Hammerstein, Wiener, and Hammerstein-Wiener architectures. To motivate our approach we first show that some already established compact circuit models can be expressed in terms of these architectures. Then, we demonstrate that nonlinear circuits with simple, scripted behaviors can be approximated well by these canonical system identification architectures without introducing unnecessary additional computational complexity. In particular, we show that parsimonious Hammerstein-Wiener models are effective surrogates for nonlinear CMOS amplifier and comparator circuits. To train these models we use a combination of DC and transient transistor-level Spice (Xyce) simulation data. We present strategies for identification of the static nonlinearity in the models and discuss identification of the linear time invariant (LTI) portion of the models from time domain data. We conclude with several simulation results showing that our data-driven compact models can accurately reproduce circuits' behavior over a wide range of input conditions and frequencies.

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Advances in material model calibration for computational solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LEARNING THE OPTIMAL PARAMETERS GOVERNING CONFLUENT TISSUES TO SHAPE THEIR EMERGENT PROPERTIES

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ABSTRACT

Confluent tissues are complex biological tissues whose macroscopic properties and behaviors are essential to understand for the advancement of knowledge in areas such as developmental biology, tissue engineering, and regenerative medicine. These tissues are commonly described as energy-based physical systems characterized by an internal energy optimization process, in which the energy function minimized by the system depends on microscopic parameters associated with each cell. It has been shown how appropriate choices of these microscopic parameters give rise to a wide and diverse expression of macroscopic behaviors, such as a rigidity transition between a liquid phase and a solid phase [1], or the formation of patterns in the tissue. To solve the inverse problem of obtaining specific material properties, these systems can be associated with an external loss function dependent on the microscopic parameters explicitly and implicitly through the minimum energy state. Here we present an innovative framework, a fully differentiable vertex model written in Google Jax to quickly and easily address the inverse problem of learning these microscopic cellular parameters to achieve a given target behavior for confluent tissues [2]. Our framework allows us to leverage bilevel optimization techniques to learn optimal parameters for these systems in order to achieve target macroscopic behavior, such as specific patterns within the tissue, like the formation of rosette structures, or specific system properties, such as liquid or solid phases, or even infer the optimal cellular parameters to match some real microscopic data. Implementing this framework in Jax allows the model to be fully differentiable, which gives us the freedom to automatically differentiate any energy or loss function with respect to any parameter of the system. Thus, our framework allows us to address inverse problems using techniques from machine learning, such as automatic implicit differentiation and equilibrium propagation, and even use GPUs and TPUs to accelerate optimization processing time. In summary, this framework opens new avenues of research leveraging these machine learning techniques for material parameter identification in developmental biology for confluent tissues.

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Advances in neural operators for scientific modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NOVEL ENSEMBLE APPROACH TO UNCERTAINTY QUANTIFICATION IN OPERATOR LEARNING

Ravi Patel[*1]*

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ABSTRACT

Operator learning is a recently developed generalization of regression to mappings between functions. It promises to drastically reduce expensive numerical integration of PDEs to fast evaluations of mappings between functional states of a system, i.e., surrogate and reduced-order modeling. Operator learning has already found applications in several areas such as modeling sea ice, combustion, and atmospheric physics. However, even in the ideal case where operator learning recovers the training data, there will be uncertainty in interpolatory and extrapolatory regimes. A useful model is one that is transparent about its shortcomings. Single point estimates, hide the broad range of models that reasonably fit training data but present vastly differing predictions. Operator learned models with uncertainty quantification (UQ) would expose users of the models to the full range of surrogate predictions. In this talk, we introduce a novel ensemble approach to UQ in operator learning and compare it to a more standard variational Bayes approach in synthetic benchmarks and a climate application.

Data-driven methods for modeling complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TIME DELAY EMBEDDINGS TO DISENTANGLE UNSTABLE PERIODIC ORBITS IN CHAOTIC ATTRACTORS

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ABSTRACT

The data-driven modeling of dynamical systems is rapidly developing, especially for fluid systems. However, many leading algorithms require high-dimensional, full-state training data, while for many real-world systems only very limited or partial measurements are available.

To address this challenge, our work employs time delay embeddings, offering a systematic approach to reconstruct an attractor from such constrained time series measurements. Specifically, we investigate the effectiveness of long-time delay embeddings in capturing
progressively intricate unstable periodic orbits (UPOs) within a chaotic system. In fluid dynamics, these orbits correspond to exact coherent structures (ECSs). The behavior of a chaotic attractor can be understood as the combination of all its periodic orbits. This is particularly relevant when studying the turbulent behavior of fluid flows, which can be represented by an infinite number of these orbits. While an infinite number of orbits are needed to fully describe the system, the dominant dynamics can be captured by the shortest, or ‘fundamental’, orbits. By finding enough of these orbits, we can make predictions about the statistical behavior of turbulent flow.

Our results show that, for long time delay embeddings, UPOs disentangle and converge to a discrete Fourier decomposition. We present an analysis for the disentanglement of these UPOs of the Lorenz attractor and Rössler attractor. The time delay embeddings obtained for these UPOs can be further used to model the dynamical system and forecast its behavior.

Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LEARNING AND ADAPTING - SECRETS TO SUCCESSFUL, MODELING, COMPUTING AND PREDICTING

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ABSTRACT

We will survey in this talk a consistent approach pioneered by Prof Oden among others of iteratively learning and adapting models that underlies many successful developments in modeling and predictive simulations. The simple questions ``how good is the model" and ``how to improve it" are answered repeatedly and consistently until a simulation fit to purpose is accomplished. We see this approach in the classical a posteriori error estimates for finite element models followed by adaptive updates to mesh and models. While, these questions are simple the answers are not! Error analysis of models is rarely a simple comparison of a few samples of ground truth to model prediction since the purpose of a model is to predict on unseen cases and often at ranges and scales beyond those observable. Similarly, strategies for model improvement presume both clear identification of model inadequacies and robust strategies to improve them.
Machine learning (ML) and predictions based on such methodologies that are transforming our approaches to challenging problems in computational simulation based predictions are but the latest of the methods that are amenable to this paradigm. I will present in this talk, development of a consistent over several decades of strategies that make this a consistent paradigm for complex physics based simulationst.

FAST MODELING OF POSTFIRE DEBRIS FLOWS FOR HAZARD RISK ANALYSIS

Abani Patra[*1] and Palak Patel*[1]

[1]*Tufts University*

ABSTRACT

Computational models that can efficiently simulate geophysical flows like debris flows and landslides are crucial for creating hazard maps that can be used to identify high-risk zones, which helps implement preventive measures (Vallis,2016). However, simulating large flows over natural terrain uses large computing and data resources. Additionally, the uncertainty in the data sources and model parameters requires large ensembles for uncertainty quantification and hazard analysis to study the behavior of such flow. To address this challenge, we present an interesting approach that first creates a deep learning surrogate model to emulate geophysical flow using a modified U-Net architecture that is effective for simulating geophysical flow for its ability to extract spatial patterns in the flow fields (Lino et al 2020). This model can be trained on large ensembles of fast-to-compute feature-rich small flow computed using our first principles code TITAN2D, a geophysical flow modeling software (Patra et al 2005). Once trained, this model can then be extended to a larger unseen terrain using only a limited number of expensive simulations building on the ideas of transfer learning. This model can be further employed to perform fast approximations of the Titan2D simulations and to explore parameters uncertainty and hazard analysis using the Monte-Carlo approach. Here we illustrate this scheme on a case study from post-fire debris flows in Southern California.

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Computational mechanobiology of musculoskeletal tissues
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE "OSTEOSTAT": AN OSTEOCYTE-BASED THEORY OF BONE MECHANOBIOLOGY

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ABSTRACT

The osteocyte network in bone is believed to play an important role for how bone tissues sense and respond to mechanical stimulation. Yet, bone adaptation to mechanical loads is often conceptualised as a simple bone optimisation response to mechanical stimuli, such as Wolff's laws, in which overloaded regions of bone are consolidated and underloaded regions of bone are removed. Such laws are based on mechanical variables only; they lead to a one-to-one correspondence between bone structure and mechanical loading, and they presume the existence of a reference mechanical state, the mechanical setpoint.

In this contribution, we extend a theory of bone tissue sensing and adaptation based on osteocytes [1] to provide new understanding of the role played by osteocyte signals in bone tissue regulation. This theory embodies the mechanical setpoint as osteocyte properties involved in mechanotransduction. It includes setpoint adaptation due to the replacement of osteocytes during remodelling, making the setpoint space and time dependent. As a result, bone structure depends on the loading history rather than the current loading state, consistently with experimental observations. Our work extends [1] by accounting for varying osteocyte populations within bone tissue, allowing us to determine osteocyte lifespan due to bone removal and cell death, and to explore bone adaptation under osteocyte disruptions, which is particularly relevant to age-related bone loss. We present numerical investigations of this new theory of bone adapation to explore how mechanobiological response curves (effective Wolff's laws) are modulated by setpoint adaptation during remodelling and by disruptions to osteocyte signals due to loss of osteocytes with age. We find that biological disruptions of remodelling balance cannot always be compensated by mechanical feedback. Our model suggests that setpoint adaptation during remodelling may have significant observable consequences, such as an increase in average osteocyte density during unloading, and hysteresis in bone response signatures that resemble lazy zones.

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Biomechanics of hard tissues: From experiments and simulations to clinical applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT AND VALIDATION OF AN OPEN-SOURCE QCT-BASED FINITE ELEMENT ANALYSIS AND PHASE FIELD MODELING FOR FRACTURE PREDICTION IN GOAT TIBIA

Debangshu Paul[1], Zachariah Arwood[1], Pierre-Yves Mulon[1], Dayakar Penumadu[1] and Timothy Truster[1]*

[1]*University of Tennessee*

ABSTRACT

Predicting mechanical responses under various load conditions is of significant interest in the field of orthopedic research. Despite an abundance of research on finite element (FE) modeling for human bones, studies specifically focusing on the tibia remain notably limited. Given that mechanical properties and structural form of goat tibias closely mimic those of human tibias, they can serve as excellent models for comparative orthopedic research. While existing literature on ovine bone research offers rich in vivo models, it lacks a validated FE model of the tibia subjected to thorough spatial error assessment.

This article presents a novel open-source-based FE model of a goat tibia incorporating phase field fracture representation. The model was validated using Digital Image Correlation (DIC)-measured strain under compression, offering a valuable tool for bone biomechanics research. A model of bone geometry was constructed from a 3D quantitative computed tomography (QCT) scan of the goat tibia. Density was calculated from Hounsfield values and spatially distributed within the FE mesh. To validate this FE model, we conducted a uniaxial compression test by applying the load along the shaft axis. A DIC system provided high-resolution strain measurements across the surface of the tibia, with results found to align well with FE simulation outcomes - thus validating our elastic model.

To quantitatively predict three-dimensional fractures, we used a high-performance computer (HPC) environment to couple our elastic model with a phase field model – resulting in fracture initiation and evolution predictions that closely mirror experimental observations. This high-fidelity QCT-based approach offers a framework for personalized modeling of human tibias enabling patient-specific analysis relating to fracture risk, implant effectiveness, and optimal treatment strategies.

Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INFLUENCE OF DEPOSIT FREEFORM SHAPE ON THE GRAIN MICROSTRUCTURE AND RESIDUAL STRESS EVOLUTION DURING WIRE-ARC DIRECTED ENERGY DEPOSITION (WA-DED) OF IN718

Santanu Paul[1], Scott Julien[1], Elizabeth Chang-Davidson[1], Ahmad Nourian Avval[1], Samuel Boese[1], Jon Gager[1], Sean Langan[2], Rumman Ahsan[2] and Sinan Müftü[1]*

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ABSTRACT

The grain structure orientation, size, and distribution play a significant role in dictating the mechanical properties, and residual stress distribution in an Additively Manufactured (AM) metal component. In temperature-based metal AM processes such as Laser Powder Bed Fusion (L-PBF), or Directed Energy Deposition (DED) techniques, the accurate calculation of the melt-pool geometry, is crucial for the evolution of grain structures, and the development of in-process stresses during and post-deposition. Accurate calculation of the melt-pool geometry is important because it improves the prediction accuracy of the temperature gradient on the solidification front. For alloys with Face or Body body-centered cubic (FCC/BCC) crystal structures, the local orientation of the temperature gradient dictates the primary dendrite growth along a specific preferable easy growth direction of the material. This phenomenon has been observed to be more dominant in the Wire-Arc DED (WA-DED) processed Inconel alloys, wherein the fabricated components have consistently shown epitaxial growth of columnar grains oriented along the build (vertical) direction. In the Finite Element (FE) based sequentially coupled thermomechanical simulations of the WA-DED process, the usual practice is to model the deposit geometry as a rectangular block. A direct advantage of this assumption is the geometrical consistency with brick elements employed during the FE analysis. However, this assumption is inconsistent with the freeform shape of the deposited track during the WA-DED process. This work explores the importance of accurate modeling of the deposit freeform shape in the thermomechanical FE simulations for the prediction of the solidification front, local temperature gradients, the evolving in-process deformations, and the post-solidification residual stress. Additionally, the importance of freeform deposit shape on the grain structure formation, the grain orientations, and grain shapes and sizes are also estimated using the recently developed Discrete Dendrite Dynamics (DDD) model [1, 2]. Note the simulations are supported by experimental measurements and tests (such as Thermocouple, XRD, and EBSD) at various stages for calibration and validation.

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PARALLEL NEWTON-KRYLOV AND QUASI-NEWTON SOLVERS FOR NONLINEAR CARDIAC MODELS

Luca F. Pavarino[*1], Nicolás Barnafi[2], Ngoc Mai Monica Huynh[1] and Simone Scacchi[3]*

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ABSTRACT

This talk focuses on preconditioned Newton-Krylov and quasi-Newton solvers for nonlinear cardiac models arising in electrophysiology and cardiac mechanics. The preconditioners considered belong to the classes of both Algebraic Multigrid Methods (AMG) and Dual-Primal Domain Decomposition, such as Balancing Domain Decomposition by Constraints (BDDC) and Dual-Primal Finite Element Tearing and Interconnecting (FETI-DP). We first study the performance of AMG and BDDC preconditioners in a Newton-Krylov solver for cardiac mechanics, varying the choice of BDDC local and coarse solvers, primal degrees of freedom, finite element degree and investigating the strong scalability of the solvers [1]. We also study alternative nonlinear solvers for cardiac mechanics where the classical Newton-Krylov method is replaced by inexact Newton-Krylov and quasi-Newton methods, varying the problem size, data magnitude and number of processors, showing in some cases a significant speed-up over the standard Newton-Krylov method [2]. BDDC and FETI-DP preconditioners with deluxe scaling can also be applied to Newton-Krylov solvers for the Bidomain model in cardiac electrophysiology where a polylogarithmic convergence rate bound can be proven and validated by parallel numerical tests, showing that the proposed parallel solvers are scalable and quasi-optimal [3].

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Multiphysics and data-driven modeling for cardiovascular biomedicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PDE-CONSTRAINED SHAPE REGISTRATION FOR COMPUTATIONAL BIO-MODELING

Aishwarya Pawar[1], Adrian Buganza Tepole[2], Colton Ross[3], Chung-Hao Lee[4] and Ming-Chen Hsu[1]*

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ABSTRACT

We propose a novel PDE-constrained shape registration algorithm to capture the elastic deformation and growth of biological tissues from imaging data. Shape registration is the process of evaluating optimum alignment between pairs of geometries through a spatial transformation function. The presented framework evaluates the optimum spatial transformation function through minimization of an energy functional which consists of a distance measure reflecting the mismatch between the shapes and hyperelastic strain energy. We carry out the registration such that the spatial mapping satisfies partial differential equations that describe linear momentum balance of growing soft tissues.

We use 3D tensor product B-spline basis functions to interpolate 3D space. Here, the movement of the B-spline control points, composed with an implicit function describing the shape of the tissue, yields the total deformation gradient field. The deformation gradient is then split into growth and elastic contributions. The growth tensor captures addition of mass, i.e. growth, and evolves according to a constitutive equation which is usually a function of the elastic deformation. Stress is generated in the material due to the elastic component of the deformation alone. Our approach follows existing finite element implementations of growing tissue, but within the isogeometric analysis framework [1]. We apply the proposed shape registration framework to study tissue expansion during skin reconstruction surgery. Here, we characterize skin growth on a porcine animal model. The registration framework is able to achieve analysis of skin growth in the complex geometries that are available from 3D photography instead of the simplified models. We also apply the registration framework to study the mechanics of tricuspid valve deformation in patients with hypoplastic left heart syndrome (HLHS) [2]. The resulting geometry will be used in a fluid-structure interaction simulation framework to help understand the key functional metrics that indicate the onset of TR in HLHS newborns. We anticipate that our PDE-constrained shape registration method will improve our understanding of biological and medical problems in which tissues undergo extreme deformations over time.

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The phase field method for fracture: Theory, numerics, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREDICTION OF PROGRESSIVE FRACTURE IN THIN MONOLITHIC AND LAMINATED GLASS PLATES WITH AN EFFICIENT RANDOMIZED PHASE FIELD MODEL

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ABSTRACT

This study utilizes a phase-field approach to analyze brittle fracture in four-point bending of monolithic and laminated glass plates. Objectives include a thorough comparison of phase-field fracture formulations for thin glass plates, evaluating dimensional reduction and mesh parameters, and validating temperature-dependent material properties for polymer foils. Acknowledging limitations in the Bourdin–Francfort–Marigo model, two additional phase-field fracture models are explored. Challenges in resolving the phase-field length-scale parameter are addressed, proposing methodologies for determining fracture energy. Despite discrepancies in crack localization, phase-field models show agreement with measured stresses and resistance in laminated glass. The study also explores the enhanced post-critical response of laminated glass, attributing it to the composite effect of stiff glass layers and compliant polymer films. This ductility makes laminated glass suitable for safety-critical applications without sacrificing aesthetics. Traditional deterministic failure models struggle to reproduce this response, leading to the introduction of a randomized model using Weibull variables for layer-wise tensile strength. Employing a dimensionally-reduced phase-field formulation, numerical simulations demonstrate the randomized model's potential, although the predicted response falls short in ductility compared to experiments. This emphasizes the importance of considering strength variability along the beam length and incorporating it into phase-field formulations for an accurate representation of laminated glass behavior

Contact and interface mechanics: Modeling and computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FRACTURE PROPAGATION ALONG CONTACT INTERFACES

Chris Pearce[1], Lukasz Kaczmarczyk[1], Andrei Shvarts[1] and Ignatios Athanasiadis[1]*

[1]*University of Glasgow*

ABSTRACT

This work focuses on an implicit computational framework for simulating crack propagation along contact interfaces and surfaces under load in three-dimensional bodies. We restrict ourselves to brittle fracture and frictionless contact and focus on numerical challenges associated with the coupling of unilateral constraints emerging from both the contact conditions and fracture criterion.
The formulation is based on the configurational mechanics framework and is solved using the finite element method. The approach utilises a monolithic Arbitrary Lagrangian-Eulerian formulation permitting simultaneous resolution of crack propagation and unilateral contact constraints. Contact is embedded in the model using the well-known mortar contact formulation.

Evolving cracks are explicitly modelled as displacement discontinuities within the mesh. Heterogeneous approximation of arbitrary order is used to discretise spatial displacements, enabling hp-adaptive refinement around the crack front and the contact interfaces traversed by the crack. The result is a holistic approach which handles issues associated with thermodynamic consistency, numerical accuracy and robustness of the computational scheme.

Several numerical examples are presented to verify the model formulation and implementation. The examples also highlight how contact pressure on surfaces traversed by cracks influence their propagation.

The approach is validated by comparison of our simulations with both academic and industrial problems, involving cracks of complex morphologies propagating along contact interfaces between multiple deformable bodies.

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Numerical modelling of composite materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

USE OF THE STRESS TENSOR FOR PLOTTING LOAD PATHS IN ORTHOTROPIC LAMINATES

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ABSTRACT

The use of pointing vectors defined by columns of the Cauchy stress tensor to plot load paths for transfer of loads in structural mechanics has been recognised for some time [1,2] and more recently verified in two-dimensional elasticity by the work of Tamijani et al [3].

The stress tensor is given by the results of a finite element analysis. It has been shown, for example in [2], that the three columns of the stress tensor are vectors that are parallel to the force flow in each of the coordinate directions. Contours parallel to these vectors define walls across which the corresponding force does not flow. Defining neighbouring contours, initiating where load is introduced to the domain, defines paths along which load is transferred. When there are no distributed forces the load transferred along the path is constant. When body forces are present, such as gravity or inertia loads in transient dynamics, the force being transferred between the walls will vary. The imagery is therefore enhanced by color coding the contours according to the magnitude of the path vector. This color coding indicates the load per unit area being transferred locally along the path.

The stresses can come from a static linear elastic analysis, or from a transient or material nonlinear solution in structures with beam, plate or solid components. Applications in [2] included force transfer through a bolted joint and transient stress propagation in a helicopter frame following impact.

This paper will focus on the three-dimensional load transfer within laminated orthotropic materials including load transfer between plies in the presence of geometric discontinuities and ply drops. The role load paths can play in optimal fiber placement will also be discussed.

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Advanced computational modelling of wood, wood-based products, bio-composites, and timber structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MACROSCALE MODELING OF WOOD FRACTURE UTILIZING THE PHASE FIELD APPROACH

Sebastian Pech[*1], Markus Lukacevic[1] and Josef Füssl[1]*

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ABSTRACT

Wood, as a naturally grown material, exhibits an inhomogeneous material structure as well as a quite complex material behavior. For these reasons, the mechanical modeling of fracture processes in wood is a challenging task and requires a careful selection of numerical methods. Promising approaches like limit analysis or the extended finite element method (XFEM) in combination with microstructure materials models deliver good but not yet satisfying results. Particularly the latter approach, including XFEM, has severe difficulties with crack paths in regions with complex morphology, mainly around knots. Therefore, in this work, the focus is laid on the recently emerging and very popular phase field method [1]. Especially geometric compatibility issues that limit the use of XFEM can be avoided, as the crack is not discretely modeled but smeared over multiple elements. This allows the formation of complex crack patterns, defined by the underlying differential equations and boundary conditions but not restricted by the mesh geometry. The present implementation [2,3] contains a stress-based split which allows proper decomposition of the strain energy density for orthotropic materials. Furthermore, the geometric influence of the wood microstructure on crack propagation is taken into account by a structural tensor scaling the length scale parameter of the phase field [3]. For solving the system of differential equations, a staggered approach with an additional Newton-Raphson loop is used. The developed algorithm was tested on various problems. Compared to XFEM more computation time was needed as the phase field method requires a finer discretization. However, crack patterns, including branching and merging, could be modeled very stable and accurately, even in the vicinity of knots where the material structure of wood is particularly complex and interface zones exist.

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Next-generation numerical methods for coupled multiphysics problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFICIENT SOLVERS FOR BIOT'S EQUATIONS

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ABSTRACT

In this work, our goal is to design efficient numerical methods for the poroelastic Biot's equations that model the soil consolidation process. Discretization of these equations yields large-sparse linear systems whose efficient solution is a key point. For the solution of Biot's equations there are two main approaches: iterative coupling methods and monolithic or fully coupled methods. Both strategies will be considered by means of several numerical methods such as the so-called fixed-stress split method and monolithic multigrid methods. Moreover, the authors will propose improved versions of these methods and show their good performance for some numerical experiments.

Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADVANCED COMPUTATIONAL MODELLING OF THE PLASTICITY OF COMPLEX METALLIC MICROSTRUCTURES - MICROSCALE VALIDATION AND MACROSCALE EXPLOITATION

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ABSTRACT

A Discrete Slip Plane model has been developed to account for the heterogeneity of plastic deformation at the subgrain scale, as well as for nonstandard, highly orientation-dependent plastic mechanisms facilitated by the substructure of some of the phases of interest. The model is founded on the concept that individual, atomic slip planes have a different likelihood of becoming active due to the presence of dislocation sources and obstacles on them. It hence considers the discrete slip on each of them and assumes it to depend on the ratio of the resolved shear stress and a slip resistance which is sampled from a statistical distribution which takes into account the presence of sources and obstacles [1].

In the numerical implementation of the model, a large number of (atomic) discrete slip planes are collected into bands, whose response is governed by the weakest of the discrete slip planes contained in them. The thickness of the bands is considered a numerical parameter. For sufficiently small values, the result is found to be insensitive to the band thickness. The resulting governing equations resemble those of conventional crystal plasticity, albeit with slip system specific and spatially varying properties. They are solved using the finite element method and fully consistent Newton-Raphson iterations.

The model has been validated against micro-tensile tests on advanced high strength steel samples which have locally been thinned to a few micron, so that their microstructure is practically uniform through the thickness. This allows us to construct finite element models which capture the full, three-dimensional microstructure of the region of interest in great detail and without the usual uncertainty on the subsurface microstructure [2]. A very good agreement between the experimental and numerical slip patterns is observed.

Simulations of three-dimensional representative volume elements of the material allow us to understand particular features of its macroscopic response, such as e.g. the very steep initial hardening observed for martensite.

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Advances in damage & fracture modeling of multiphysics materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HYDRAULIC FRACTURE RECESSION IN A POROUS MEDIUM: THE SUNSET SOLUTION

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ABSTRACT

Abstract
There has been considerable research devoted to modeling fractures driven to propagate in a porous elastic medium by the injection of a viscous fluid. Once fluid injection ceases, the fracture may, depending on the dominant process among the multiple competing physical processes, continue to propagate till arrest or arrest immediately, deflate without changing its footprint, and then finally recede due to the loss of fluid to the porous medium. Recent analytic work [1] has established the tip asymptotics for receding hydraulic fractures that close due to leak-off to the permeable medium as well as the multiscale asymptotes that govern the arrest-recession transition. These multiscale asymptotic results have enabled the development of rigorous numerical schemes to explore the recession dynamics of plane strain and radially symmetric hydraulic fractures [2]. These detailed studies have made possible the identification [3] of the so-called Sunset Solution, which is a similarity solution that emerges close to the ultimate collapse of the fracture. The asymptotic analysis performed in [3] establishes that the existence of the Sunset Solution is due to a fundamental decoupling of the kinematics from the dynamics in the governing equations, which leads to a robust way to measure the Carter leak-off coefficient from the rate of change in the fracture aperture at the wellbore.

In this talk we will outline the derivation of the receding asymptote and provide numerical evidence for the similarity solution that emerges close to the ultimate closure of the fracture. We will derive a particularly simple analytic expression for this Sunset Solution and demonstrate how it can be used to estimate the so-called Carter leak-off coefficient from aperture closure measurements, which characterizes the porous medium.

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Constitutive modeling of complex materials with machine learning and artificial intelligence
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AUTOMATED CARDIOVASCULAR CONSTITUTIVE MODEL DISCOVERY AND UNIVERSAL FINITE ELEMENT ANALYSIS IMPLEMENTATION

Mathias Peirlinck[*1], Denisa Martonova[2], Juan Hurtado[3], Sigrid Leyendecker[2], Kevin Linka[4] and Ellen Kuhl[5]*

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ABSTRACT

Quantifying the biomechanical behavior of cardiovascular tissues holds immense potential to enhance our understanding of (i) smooth and cardiac muscle cell responses to mechanical cues and (ii) how structural and compositional alterations within these tissues impact their overall functional behavior. Such insights are crucial to unravel disease mechanisms (e.g. atherosclerosis, aneurysm, myocardial infarction), to optimize and personalize current treatment strategies (e.g. annuloplasty ring or stent sizing), and to develop novel medical devices (e.g. artificial heart valves or vascular grafts). Such studies depend critically on the accuracy of the underlying constitutive models, which govern the thermodynamically consistent relationship between the tissue's deformation and internal stress state. Given cardiovascular tissue's highly non-linear, transverse isotropic or even orthotropic mechanical behavior and a vast ever-increasing library of potential constitutive models, identifying the most accurate material model can be a challenging procedure prone to significant user bias. To resolve this subjectivity and democratize computational engineering analysis for all, we leverage constitutive artificial neural networks and machine learning to automate and democratize constitutive model discovery for these intricate materials. Based on arterial and myocardial biaxial tensile and triaxial shear testing data, our framework autonomously identifies the optimal material models and parameters from a library of over 232 = 4,294,967,296 possible material models. By seamlessly integrating the discovered material models into a universal material subroutine for (in)compressible (an)isotropic tissues, our work advances the implementation of these models into cardiovascular finite element simulations. This not only enhances user-friendliness and robustness but also mitigates the vulnerability to human error. The automated approach signifies a significant stride towards a more inclusive, user-friendly, and accurate framework for cardiovascular biomechanics simulations, ultimately contributing to improved medical treatments for cardiovascular diseases.

Modeling friction and wear
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ELASTOPLASTIC IMPACT OF SPHERE ON LARGE PLATE

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ABSTRACT

Impact of a sphere on a plate has been recognized as a fundamental problem in contact dynamics, which couples the nonlinear contact between the sphere and the plate and the energy dissipation by the flexural wave on plate. For an elastic contact, the dynamics can be formulated using a highly nonlinear ordinary differential equation (Zener's equation), which cannot be solved exactly but only be approximated. However, elastic contact suggests low-speed impact, which is rather rare in engineering application. For a high-speed impact, both the flexural wave and the contact plasticity account for the loss of kinetic energy. Therefore, we must take the contact plasticity into account, which introduces to the problem not only more complexities, but also loading-unloading asymmetry. In this work, we modeled the elastoplastic dynamics between the sphere and plate by bringing the MYC plastic contact model into Zener's equation. With dimension analysis, this model can be controlled by only two nondimensional parameters. Solving the present equation via analytical and empirical methods, this model can accommodate the elastic impact, the fully plastic impact, as well as the transition in-between.

Transport phenomena in micro/nanofluids
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TRANSPORT AND DISPERSION OF ACTIVE COLLOIDS IN PERIODIC DOMAINS

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ABSTRACT

Transport and mixing within suspensions of swimming microorganisms are important for the understanding of many biological and industrial processes, such as infection by motile bacteria or the formation of biofilms. Different from passive particles, the ability of active swimmers or particles to self-propel gives rise to interesting dynamics including accumulation at confining boundaries and upstream swimming in the presence of a pressure-driven flow. Such unusual phenomena are a consequence of the non-equilibrium nature of active matter.

Transport and dispersion of self-propelled or active Brownian colloids often takes place in applied flows and confining boundaries. In this talk, I will present a theoretical and computational framework—the generalized Taylor dispersion (GTD) theory—that allows us to characterize the long-time drift and dispersion of active colloids in the presence of flows through periodic domains such as corrugated channels and periodic porous media. GTD allows us to reduce the Smoluchowski equation that governs the spatial-temporal evolution of the particle dynamics in its full position orientation phase space into a couple of macrotransport equations that apply at long times. The long-time transport coefficients are obtained by taking appropriate statistical moments. In pressure-driven flow through flat channels, we show that active particles can swim upstream and exhibit non-monotonic dispersion behavior in contrast to the monotonic flow-enhanced dispersion of passive matter. These predictions are consistent with those observed in experiments and Brownian dynamics (BD) simulations. Upstream swimming of bacteria poses a clinical threat in introducing catheter-associated urinary tract infection. Leveraging this theoretical and computational framework, we designed a catheter tube with internal periodic protrusions that are shown to reduce upstream swimming, and thus reduce infections by 1-2 orders of magnitude. With a prescribed pressure gradient, we calculate the flow field and the particle dynamics in the flow using a mixed continuum-BD approach. Computational results are validated against experimental measurements using 3D-printed catheter models.

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Virtual elements for partial differential equations on polytopal meshes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ARTIFICIAL NEURAL NETWORK EVALUATION OF GEOMETRIC CONSTANTS IN POLYTOPAL ELEMENT METHODS

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ABSTRACT

We presents an application of Artificial Neural Networks (ANNs) for the evaluation of geometric constants associated with polytopal element methods designed for solving partial differential equations. The constants under consideration play a key role for the numerical methods considered, impacting areas such as, among other things, a posteriori error estimates and method-specific stabilization parameters.
Leveraging ANNs, our methodology focuses on learning the dependencies between these constants and the geometric metrics of polytopal elements.
The algorithm's primary costs are confined to data processing and learning phases, that can be performed offline once and for all, resulting in an efficient method for computing the constants.

Numerical modelling of composite materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SIMULTANEOUS ENERGY HARVESTING AND SENSING USING PIEZOELECTRIC ENERGY HARVESTER BASED ON METAMATERIAL-INSPIRED STRUCTURES

Patricio Peralta-Braz[*1], Mehrisadat Makki Alamdari[1], Elena Atroshchenko[1] and Mahbub Hassan[1]*

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ABSTRACT

Piezoelectric Energy Harvesters (PEHs) are devices that enable taking advantage of the mechanical energy available in various sources of vibrations, transforming it into electrical power to supply low-power devices autonomously. Efficiency plays a critical role in these technologies, which depends strongly on achieving close synchronisation between the resonance frequency of the harvester and the source. On the other hand, there has been a growing interest in utilising these devices as sensors to acquire information about the source of vibration. Integrating these functions simplifies system design and optimises energy usage by efficiently directing generated energy to power other system components, such as a transceiver for cloud-based data transmission. This study introduces a novel design for Piezoelectric devices based on a Metamaterial-Inspired Structure for Simultaneous Energy Harvesting and Sensing (SEHS) system, aiming to enhance efficiency and power generation at low frequencies. The dynamic behaviour of the devices is modelled based on the Kirchhoff-Love plate theory and Hamilton's principle. Isogeometric Analysis (IGA) is used to solve the problem due to its capability to represent exactly complex geometries. Metamaterial-inspired structures often require multiple patches for representation, and to address this, Nitsche's method is incorporated. This method effectively manages C0-continuity and imposes conditions on the continuity of Dirichlet and Neumann's boundary conditions across interfaces. A machine learning framework is presented to infer relevant information from a highway bridge. It comprehensively describes the framework, including its key components and methodology. This study provides a valuable tool for designing and optimising SEH systems based on metamaterial-inspired structures, opening new avenues for practical applications. Numerical studies are conducted to assess the performance of metamaterial-inspired devices compared to traditional configurations.

Towards predictive digital twins: Innovative algorithms for physics-, data-assisted and hybrid modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HYBRID FINITE-ELEMENT / NEURAL-OPERATOR MODELING OF ICE-SHEET DYNAMICS

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ABSTRACT

Modeling the dynamics of Greenland and Antarctic ice sheets is critical to provide probabilistic projections of sea-level rise. In order to accurately quantify the uncertainty of the sea-level projections due to uncertainty in the model parameters, we need to run the ice-sheet models for a large number of parameter samples, which is often infeasible due to the cost of ice-sheet computational models. To address this issue, we propose a hybrid approach to approximate existing finite-element ice-sheet models at a fraction of their cost. In this approach, the finite-element model for the ice momentum equations, which is the most expensive part of an ice-sheet model, is replaced by a Neural Operator, while the classic finite-element discretization for the evolution of the ice thickness is retained. We demonstrate the approach modeling the Humboldt glacier in Greenland. We show that the hybrid model is accurate and an order of magnitude faster than the traditional finite-element model. The hybrid model can provide statistics of the glacier mass loss that are in agreement with those computed using the reference finite-element model. For increased accuracy, the hybrid model can be effectively used in a multi-fidelity strategy where a relatively small number of evaluations of the finite-element model (considered the high-fidelity model) are used together with evaluations of the hybrid model to improve the projection of the glacier mass loss.

Current trends in phase-field modeling and computations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHASE-FIELD MODELING OF BRITTLE FRACTURE UNDER CYCLIC LOADING: A NEW GRADIENT-BASED ENERGY SPLIT CRITERION

Umberto Perego[*1], Ayrton R. Ferreira[2] and Alessandro Marengo[3]*

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[2]*University of São Paulo*
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ABSTRACT

In this work we propose a computationally effective new criterion to avoid crack propagation under prevailing compression states due to load reversal in phase-field modeling of brittle fracture. In classical approaches the elastic energy is split into ‘active’ and ‘passive’ components. The ‘active’ ones enter into the phase-field driving force, whereas the ‘passive’ ones do not. The most popular approaches are probably the volumetric-deviatoric split, and the spectral split. For a summary of existing approaches along with a new proposal, see the recent work [1] and the references therein.
Making use of a simple example, similar to the one proposed in [1], we show the limitations of the volumetric-deviatoric and of the spectral energy splits. To overcome the problem, we simply propose to eliminate the contribution of the elastic energy from the phase-field driving force in those regions where the stress state is promoting crack closure. This is obtained by identifying the crack direction based on the current phase-field distribution and by computing the sign of the normal stress component in this direction. This in line with what has been proposed by other authors (see, e.g. [2]).

The formulation is based on two assumptions. The first one is the identification of the normal-to-crack direction with the damage gradient direction [2]. The second assumption consists of considering the sign of the projection of the stress tensor on the normal-to-crack direction at a point as an indicator of whether at this point the crack is opening or closing. In the first case, the whole elastic energy is ‘active’ and contributes to the crack driving force. In the second case, it is ‘passive’ and it does not contribute.

The accuracy of the present model under cyclic loading is assessed by means of the analysis of several benchmark problems. The obtained results confirm that the proposed energy split matches classic crack propagation predictions under tensile loading for Mode I and II, confining crack propagation to points subjected to prevailing tensile states while recovering the intact stiffness upon load reversal.

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SOLUTION-ACCELERATION VIA HYBRIDIZATION OF FLUX RECONSTRUCTION METHODS

Carlos Pereira[*1] and Brian Vermeire*[1]

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ABSTRACT

Resolving complexities that characterize flows of practical engineering applications often poses significant challenges to numerical simulations. These challenges arise from a large number of degrees of freedom required to resolve the underlying physics accurately. High-order methods offer increased accuracy with reduced computational cost per degree of freedom. Among these methods, the Flux Reconstruction (FR) [1] approach is able to recover existing formulations, such as Discontinuous Galerkin (DG), via correction functions.

FR methods have proven effective in handling industrial flows governed by the Euler and Navier-Stokes equations on complex geometries. These type of problems typically involve grids with localized regions of stiffness introduced by the element size, which limit the maximum allowable time-step size in explicit time stepping. On the other hand, the computational cost of implicit time discretizations, associated with solving nonlinear systems that require linearization and preconditioning, scale with (p + 1)^d for a given spatial order p+1 and problem dimension d.

Hybridization of high-order methods, as pioneered by Cockburn et al. [2] DG methods and further extended to FR by Pereira and Vermeire [3], can be used to reduce computational cost of implicit discretizations. By introducing a trace variable and a global conservation statement, hybridization effectively reduces the scaling of the implicit system down to that of a lower-dimensional problem, typically allowing for smaller problems that require reduced computational cost.

Purely implicit methods remain computationally expensive for practical problems with increased numerical stiffness even after hybridization. In this sense, Implicit-Explicit (IMEX) integration can reduce geometry-induced stiffness by partitioning using an implicit method in regions of high geometry-induced stiffness and larger elements with an explicit method. Pairing hybridized and standard FR methods for the implicit and explicit portions, respectively, enables a significant reduction of computational cost over purely explicit methods. We demonstrate how hybridization can be used as a solution-acceleration technique to enable faster results without sacrificing accuracy. Results are illustrated via a series of numerical examples, including turbulent flow over a multi-element airfoil, showcasing speedup factors up to 50 times.

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Numerical modelling of composite materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPARATIVE ANALYSIS OF PGFRP COOLING TOWER STRUCTURAL CONFIGURATIONS

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ABSTRACT

Pultruded glass fiber reinforced polymer (pGFRP) profiles are light, strong and corrosion resistant, and for decades have been used in large frame structures such as cooling towers. In this type of structure, it is common to use channel beams eccentrically connected to square hollow section (SHS) columns by a single bolt, which allows for easy assembly and savings in terms of connecting hardware. However, little is found in scientific literature about their structural performance. The current study assesses the structural behavior of this type of structure and compares it to a cooling tower designed as a traditional steel structure with I-beams and wide flange columns. The design of the structures is based on the Brazilian pre-standard for pultruded composite structures and finite element (FE) models were developed in the software SAP2000. The comparison is based on the total weigth, natural frequencies and quantity of materials, with the aim of stating the most optimized configuration for cooling towers made of pultruded composite material.

Mesh-free particle methods for multi-physics problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A STUDY ON THE EFFECTS OF SOLIDITY RATIO ON VIRTUAL GRATING MODELING OF WAVE-SLAT INTERACTION

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ABSTRACT

The wave impact on coastal and offshore structures can lead to damages or stability issues. Aiming to mitigate the wave-induced loads, wave breakers that allow partial water circulation are effective. An example is the grating with a set of thin inclined slats, in which flow deflection may occur, depending on the angle of attack. Considering that the hydrodynamics can be affected by tiny spacing between the slats, the analysis of the effectiveness of such grating structures usually involves different spatial scales. As most particle methods, which are very effective to simulate highly nonlinear fluid structure interactions with free surface piercing structures, employ a single uniform resolution across the entire computational domain, the simulations of multi-scale Wave-Structure Interactions (WSI) problems requires a considerable number of particles to model both the fluid and solid domains. A computationally cost-saving alternative to model the effects of flow deflection due to the inclined slats is the adoption of the Virtual Grating (VG) technique. In the VG, the grating structure is modeled as a control volume and the particles' velocity normal to the slats inside the region are set to zero, reproducing the effects of the inclined slats. In the present work, the effects of the grating solidity ratio on the accuracy of the VG technique are investigated through simulations of wet dam break. For this purpose, the VG was implemented in an in-house projection-based Moving Particle Semi-implicit (MPS) framework, herein called MPS-VG. To verify the results obtained by the MPS-VG, simulations using the conventional particle-based MPS modeling are also performed. As a result, the correction factor for the deflection angle as a function of the solidity ratio is obtained.

Keywords: Grating, inclined slats, solidity ratio, Virtual Grating, Moving Particle Semi-implicit

Accelerating failure predictions through advances in scientific machine learning and scientific computing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE MESH-BASED GRAPH NEURAL NETWORKS WITH ADAPTIVE MESH REFINEMENT FOR PHASE FIELD FRACTURE PROBLEMS

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[1]*Auburn University*

ABSTRACT

Phase field (PF) methods, coupled with adaptive mesh refinement (AMR), have been widely used to study crack propagation in materials due to their robust formulation and ease of implementation. Despite their advantages and recent advancements in scalable implementations, PF fracture simulations can be slow and expensive, limiting their adoption in high-throughput applications. Mesh-based graph neural networks (GNNs) have shown promise in engineering problems involving complex physics on a mesh. However, mesh-based GNNs suffer from over-smoothing in problems involving very fine meshes due to a large number of required message-passing steps.

In this work, we develop a dynamic multiscale mesh-based GNN formulation for multiphysics problems with AMR. We use this approach to study PF-fracture problems using block-structured AMR (BSAMR) in brittle materials under tension and shear loads. We construct graphs using meshes of different resolutions where mesh points act as graph nodes and mesh edges act as graph edges. The proposed mesh-based GNN approach mimics a conventional iterative multigrid solver and applies a series of downsampling (coarsening) and upsampling (refining) steps on encoded feature vectors. We use skip-connections to connect similar levels at downsampling steps and upsampling steps to transfer information. The proposed approach mitigates problems of over-smoothing by linking points in fine-resolution regions over longer distances. Next, we propagate the solution in time and identify areas for mesh refinement. We perform BSAMR by inserting nodes (or mesh points) and edges (or mesh edges) and updating the graphs at corresponding levels.

We used this approach to simulate Mode-I and Mode-II fractures in brittle materials. First, we generated the training dataset for Mode-I crack using physics-based PF fracture simulations on a square domain with a crack (of different lengths and angles) on the left edge. We trained the dynamic multiscale mesh-based GNN on these simulations, performed validation studies, and tested the GNN framework for accuracy and performance. Next, we optimized the framework's architecture for optimal speed and accuracy. Finally, we used transfer learning (TL) to extend the framework to Mode-II loading and new crack locations within the domain. The framework demonstrated excellent accuracy and speedups compared to physics-based PF fracture simulations.

Novel mathematical and numerical models for multiphysics and multiscale systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOWARDS ANATOMICAL POROMECHANICAL MODELS OF THE RESPIRATORY SYSTEM FOR PERSONALIZED MECHANICAL VENTILATION IN RESPIRATORY FAILURE

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ABSTRACT

Mechanical ventilation is a double-edged therapy in which objectives such as relieving the work of breathing, improving gas exchange, and avoiding alveolar overdistension must be balanced to sustain life. Determining the appropriate ventilator configuration is challenging as inter-subject variability is large and comorbidities are frequent. The development of personalized therapies may help optimize the clinical outcome. Computational lung models can be tailored to the patient's physiology, offering insight into their pulmonary mechanics across different scales.

While applications of lung models continue to emerge, validation against clinical data remains scarce, often presented only as proof of concepts. In this work, a novel computational model is formulated and validated using experimental data during mechanical ventilation. We develop a non-linear poromechanical model of the lung parenchyma coupled with a 0D model of flow across the patient's airway tree, using patient-specific geometries extracted from CT images and based on the work of Avilés-Rojas and Hurtado (2022) and the coupling approach of Berger et al. (2016). This approach simulates the lung's response to mechanical ventilation stimuli and assesses its predictive capabilities. Our approach is validated using previous studies' porcine data of volume-control ventilation experiments. Two validation approaches are employed: (i) the global model response is compared against experimental respiratory mechanics signals during volume-control ventilation. (ii) the end-inspiratory model prediction for the porosity distribution is compared against end-inspiratory CT data using regional aeration histograms.

By assessing the gap between the numerical predictions and actual lung behavior, we aim to guide future research endeavors. Our ultimate goal is to provide a clinically robust model to contribute to developing personalized mechanical ventilation therapies.

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Recent advances in high-order methods for computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMPLICIT SHOCK TRACKING FOR HIGH-SPEED FLOWS WITH ATTACHED SHOCKS

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ABSTRACT

Shock tracking aims to generate a mesh such that element faces align with shock surfaces and other non-smooth features to perfectly represent them with the inter-element jumps in the solution basis, e.g., in the context of a finite volume or discontinuous Galerkin (DG) discretization. These methods lead to high-order approximations of high-speed flows and do not require nonlinear stabilization or extensive refinement in non-smooth regions because, once the non-smooth features are tracked by the mesh, the high-order solution basis approximates the remaining smooth features. Implicit shock tracking methods recast the geometrically complex problem of generating a mesh that conforms to all discontinuity surfaces as a PDE-constrained optimization problem. The optimization problem seeks to determine the flow solution and nodal coordinates of the mesh that simultaneously minimize an error-based indicator function and satisfy the discrete flow equations.

For problems with shocks attached to surfaces, implicit shock tracking requires nodes to slide along surfaces of the object, which can be challenging for complex geometries. In this work, we develop a parametric description of surfaces of the domain from a high-order surface mesh and directly optimize the parametric coordinates of each surface node in the shock tracking setting. This ensures all surface nodes will conform to their original boundaries throughout the optimization procedure, and successfully produces shock-aligned meshes for flows with attached shocks.

Multiscale computational and data-driven approach of advanced materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN SCALE-BRIDGING APPROACHES FOR COMPLEX ALLOYS

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ABSTRACT

The extremely large compositional space of complex alloys such as High Entropy Alloys (HEA) promises the development of highly tailored materials solutions with unique combinations of properties. However, the correspondingly astronomically large configurational space of local atomic environments makes the predictions of mesoscale materials properties, such as radiation resistance or elasto-plastic response, from atomistic simulations extremely challenging.

We present a comprehensive computational framework to accelerate the development of atomistic-to-mesoscale scale-bridging models through i) physics-informed machine learning to learn how the properties of local atomic environments affect the response of the material, and ii) uncertainty-quantification (UQ) to guide the generation of additional atomistic data to optimally inform the mesoscale models. We present two examples, the prediction of defect transport coefficients and the development of flow rules for crystal plasticity, that were autonomously developed using a large-scale computational framework guided by UQ. This approach offers a promising avenue to exploit massive scale computing to assist the exploration of the chemical space of HEA for specific applications.

Deep and machine learning methodology in the context of application to computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

POLYGONAL MESH GENERATION WITH OPTIMAL CONNECTIVITY USING DEEP REINFORCEMENT LEARNING

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ABSTRACT

We consider the task of generating polygonal meshes for straight-sided geometries using a machine learning approach. We only allow for a set of basic mesh edit operations, namely edge insertion/deletion and vertex insertion/deletion. The objective function is a combination of the desired degree of the vertices as well as the faces (that is, the number of sides of the polygonal element). This allows us to generate for example fully triangular or quadrilateral meshes, by simply specifying the desired face degrees 3 or 4. At the boundary nodes we employ a heuristic which is aimed at producing high-quality final meshes. A deep neural network is applied to the half-edge data structure of the mesh, and it is trained on randomly generated geometries using reinforcement learning. We demonstrate the performance of the framework, and show the generation of nearly optimal meshes with triangular, quadrilateral, or higher polygonal elements. We also consider the benefits of introducing the element qualities into the objective function.

Recent advances in high-order methods for computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A HALF-CLOSED DG-SEM METHOD FOR WAVE PROPAGATION AND FLUID DYNAMICS

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ABSTRACT

We present a Discontinuous Galerkin Spectral Element Method (DG-SEM) with half-closed nodes and demonstrate its benefits for problems such as time-domain wave propagation and the compressible Navier-Stokes equations. For quadrilateral elements, we use one-sided Gauss-Radau points to obtain one additional degree of quadrature precision over the commonly used Gauss-Lobatto nodes. This results in an exact and diagonal mass matrix, and less aliasing error for convection dominated problems. Compared to Gauss-Legendre nodes, our scheme produces fewer connectivities and in particular generates a sparsity pattern similar to continuous Galerkin methods. For triangular elements, we develop half-closed nodesets that have optimal quadrature degrees as well as sparse interpolation operators for any additional quadrature nodes. We use this to develop efficient implicit solvers based on static condensation and iterative preconditioners operating on smaller blocks than traditional DG.

Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE CHEMO-THERMO-HYGRO-MECHANICAL BEHAVIOUR OF BLENDED CONCRETES AT ELEVATED TEMPERATURES

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ABSTRACT

Cement is one of the largest global CO2 emission sources worldwide. Replacing ordinary Portland cement clinker with silica fume, fly ash or other supplements can reduce the enviromental impact up to 50%. However, this contemporary cements show higher explosive spalling risks under fire loading in experiments. Although, the origin of this behaviour is still unclear, the drying front of concrete under fire loading was identified as important influence on the spalling behaviour. Due to the variety of blended concrete compositions, experimental investigations of the drying front are very costly. Computational models offer a possible remedy to capture the drying front for a variety of blended concretes and can lead to important insights into the problem's specifics with its multiphysical nature.

Based on chemo-thermo-hygro-mechanical analyses, the drying front of blended concretes under fire loading is investigated at macro scale, considering four primary state variables, i.e., gas pressure, capillary pressure, temperature, displacement and two internal variables, i.e., dehydration degree, chemo-mechanical damage.

A stochastic model employing Arrhenius equations for each cement constituent is utilised to quantify the dehydration degree for different blended concretes. The initial volume fractions of the studied cement composition are determined through a hydration model. Subsequently, the water release, porosity increase, and Young’s modulus of the hardened blended cement paste under elevated temperatures are coupled with the dehydration degree through established stoichiometric chemical dehydration formulas and Eshelby-type homogenisation.

Utilising a micro-poro-mechanical framework, the localisation of chemo-thermo-mechanical damage and stress states is achieved through Eshelby-type homogenisation techniques across various observation scales - concrete, mortar, and cement paste. Macroscopic stresses and the thermal incompatibility between aggregates and hardened cement paste induce stresses at different levels. At the cement paste scale, localised stresses drive thermo-mechanical damage, characterised by the expansion of randomly distributed and oriented penny-shaped inclusions. The chemo-mechanical damage is captured by dehydration induced porosity in both cement paste and aggregates.

Blended concretes, namely CEM II/A-LL, CEM III/B, CEM II/B-V, CEM II/B-Q, are analysed in the context of a numerical sensitivity study comparing the calculated drying fronts. It turns out that the grinding fineness and the hydration degree, both of which mainly determine the initial permeability, have a major influence on the drying front. Moreover, the monosulfoaluminate, ettringite and C-S-H volume fraction mainly determine the water release of cement paste due to dehydration, which also affects the drying front.

Geomechanics of the cryosphere
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMPLEMENTATION OF THE MATERIAL POINT METHOD ON A SPHERICAL VORONOI MESH FOR THE MPAS-SI-MPM SEA ICE MODEL

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ABSTRACT

Sea ice plays an important role in the global climate by reflecting solar radiation and influencing ocean circulation making it essential to accurately simulate sea ice dynamics in the coupled Earth system. In this talk we describe a new Material-Point-Method (MPM)-based discretization for sea ice being implemented within the Model for Prediction Across Scales (MPAS)-Seaice framework in the Energy Exascale Earth System Model (E3SM) [1,2]. The MPAS-SI-MPM model couples Lagrangian particles with an efficient mesh-based solution of the equations of motion. Lagrangian particle methods have certain advantages over Eulerian grid-based methods for sea ice modeling due to their ability to naturally handle advection, maintain a sharp ice edge, and capture large deformations, but require additional algorithms for locating the particles on the mesh and mapping values between the mesh and particles. The salient feature of MPAS is the use of unstructured Voronoi meshes. The unstructured Voronoi meshes are Spherical Centroidal Voronoi Tesselations (SCVTs) which allow for both quasi-uniform discretization of the sphere and local refinement. The MPM implementation within MPAS requires an adaptation to this spherical Voronoi mesh. We will describe our implementation, which couples a reference element formulation of Wachspress shape functions with an element local mapping to the sphere [3], show that components of the algorithm converge as expected, and demonstrate performance on standard test cases.

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Advances in neural operators for scientific modeling
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SOLUTION OF RIEMANN PROBLEMS WITH REAL CHEMISTRY FOR COMPRESSIBLE FLOWS USING NEURAL OPERATORS

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ABSTRACT

Deep operator networks (DeepONet) constitute a class of neural network models designed to acquire the mapping between input and output spaces. For this study, we used DeepONet to solve the Riemann problems for compressible flows. In particular, DeepONet is trained to map the initial pressure ratio in a Sod problem to final time profiles of density, velocity, and pressure for low to very high-pressure ratios. Additionally, we examine Riemann's problems incorporating real chemistry, in which the output encompasses the density of chemical species in addition to pressure and velocity. The DeepONet inferred solution also satisfies physical constraints such as mass and momentum conservation as well as entropy conservation. The primary advantage of DeepONet is, after training, swiftly acquire the solution from previously unseen input data within a fraction of a second.

Uncertainty quantification and scientific machine learning for predictive modeling of complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

REAL-TIME AERODYNAMIC LOAD ESTIMATION FOR HYPERSONICS VIA STRAIN-BASED INVERSE MAPS

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ABSTRACT

We present an efficient inverse formulation for estimating aerodynamic pressure loads on a hypersonic vehicle using a strain-based sensing strategy. Real-time characterization of aerodynamic loads is critical for guidance, navigation, and control applications. In hypersonic flight environments, direct measurement of these quantities of interest is often intractable due to the harsh aerothermal conditions. Our work targets the hypersonic environment by employing strain-based sensing to infer the aerodynamic surface loads from sparse measurements of structural strain, first introduced in [1]. The strain response induced by the aerodynamic loads is governed by the partial differential equations (PDE) of linear elasticity, leading to a PDE-constrained inference problem. In our work [2], we pose the inference task as a least-squares problem with a high-dimensional linear constraint arising from a finite element discretization of the governing PDE. Due to the linearity of the constraint, a closed-form solution is available via the normal equations, which provides an inverse map from strain measurements to the aerodynamic pressure quantities of interest. Pre-computation of the inverse map, which comprises the high-dimensional system matrices, enables real-time evaluation of the least-squares solution (estimator) for a given strain measurement. The estimator is formulated for both (1) a parameterization of the surface pressure field via the proper orthogonal decomposition, and (2) a high-dimensional discretization of the surface pressure field. We employ a data-driven prior for regularization, constructed using computational fluid dynamics solutions of the surface pressure field. Additionally, the analytical covariance of the estimator provides explicit uncertainty quantification in the presence of sensor noise. The uncertainty statistics are used to formulate an optimal experimental design problem to identify the sensor configuration from a set of candidate sensors that minimizes the desired information criteria of the estimator covariance matrix. Numerical studies are conducted using the Initial Concept 3.X (IC3X) conceptual hypersonic vehicle. The results demonstrate the estimator performance for surface pressure reconstruction, as well as the corresponding force and moment coefficients, for a given noise level. We provide a discussion of accuracy, uncertainty, regularization, and optimal sensor placement for the IC3X testbed problem.

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AN OPEN-SOURCE BENCHMARK FOR TRUSTWORTHY HIGH-DIMENSIONAL SYMBOLIC REGRESSION FOR ENERGETIC MATERIALS

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ABSTRACT

Symbolic regression requires heuristic searches of the expression trees to obtain mathematical expressions that optimize performance. These searches often suffer from the curse of high dimensionality and make the generation of mathematical expressions with more than one dimension difficult. This talk introduces and benchmarks strategies that leverage both the expressivity of deep neural networks and the interpretability of symbolic equations to discover underlying equations of state for energetic materials. In particular, we introduce an open-source framework in which a variety of mathematical models are inferred from a dataset obtained from molecular dynamics. We then compare the divide-and-conquer technique enabled by neural additive models and neural kernels to reduce the dimensionality of the symbolic regression problems with classical symbolic regression benchmarks based on genetic programming. Special emphasis is placed on (1) the approach to enforce physical compatibility (e.g., material frame indifference, material symmetry, thermodynamics) and (2) the predictive and descriptive accuracies of the models. Finally, the implications of the lack of universally accepted metrics, as well as the lack of open-source third-party validation to measure the interpretability and accuracies of the learned models, will be addressed.

Multiscale methods for advanced manufactured materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DYNAMIC BEHAVIOR OF RIBBED VISCOELASTIC CNT-PDMS THIN-FILMS FOR MULTIFUNCTIONAL APPLICATIONS

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ABSTRACT

Tailored ribbing structures were obtained by large-scale rolling in polymer thin-films by adding CNT inclusions, which significantly improved the mechanical behavior of systems subjected to dynamic compressive strain rates. A nonlinear explicit dynamic three-dimensional finite-element (FE) scheme was used to understand and predict the thermomechanical response of the manufactured ribbed thin-film structures subjected to dynamic in-plane compressive loading. Representative volume element (RVE) FE models of the ribbed thin-films were subjected to strain rates as high as 10000/s in both the transverse and parallel ribbing directions. Latin Hypercube Sampling of the microstructural parameters, as informed from experimental observations, provided the microstructurally based RVEs. An interior-point optimization routine was also employed on a regression model trained from the FE predictions that can be used to design ribbed materials for multifunctional applications. The model verifies that damage can be mitigated in CNT-PDMS systems subjected to dynamic compressive loading conditions by controlling the ribbing microstructural characteristics, such as the film thickness and the ribbing amplitude and wavelength. This approach provides a framework for designing materials that can be utilized for applications that require high strain rate damage tolerance, drag reduction, antifouling, and superhydrophobicity.

AN ALTERNATIVE ANISOTROPIC PLASTICITY MODELING APPROACH USING A SURROGATE ISOTROPIC MODEL AND STRONGLY TYPED-GENETIC PROGRAMMING-BASED SYMBOLIC REGRESSION

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ABSTRACT

Interpretable machine learning has been used to train continuum plasticity models in a range of applications. While interpretable, these models must still be implemented for material- or structure-scale simulations (e.g., within a finite element solver), which can require considerable domain knowledge. To automate this process, an alternative approach is presented where an arbitrary anisotropic yield surface is mapped to a surrogate isotropic model. In this way, only a surrogate isotropic model needs to be implemented within a finite element solver, and the mapping is learned via interpretable machine learning. Such a method could potentially lower the technical barrier for modeling anisotropic yield behavior or automatically generate models from large sets of experimental data in high-throughput scenarios.

In this presented approach, a mapping between an anisotropic yield surface and the surrogate isotropic surface is provided as input to the implemented constitutive model. The approach is based on the work of Oller et al. [1], who used the transformed-tensor method to map an anisotropic yield criterion to a “fictitious” isotropic yield criterion. That method was recently extended by Randall [2] to determine the requisite transformation tensors as a function of evolving state variables (e.g., plastic strain) using strongly typed-genetic programming-based symbolic regression (ST-GPSR).
In this work, a proof-of-concept for the presented approach is demonstrated and evaluated. Using recent modifications to the GPSR code BINGO [2,3], transformation tensors mapping anisotropic yield surfaces to a surrogate isotropic surface are obtained for examples with varying complexity. These mappings are provided to a surrogate isotropic yield model implemented within a finite element solver. Finite-element simulations are performed, where the results from the presented mapping approach are compared and benchmarked against finite-element results for which the anisotropic yield behavior is explicitly implemented. The results from this study are expected to determine the efficacy and potential downfalls of the presented approach.

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Advanced materials and smart structures: Modeling, simulation and testing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CORRELATION BETWEEN SURFACE-TO-VOLUME RATIO OF THE PARTICLE SHAPE AND ELASTIC PROPERTIES OF THE PARTICULATE COMPOSITES

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ABSTRACT

Presented studies are motivated by real-world particle shapes, observed using a scanning electron microscopy.
The focus of the presented studies was to understand the effects of the particle shapes on the effective elastic properties of the two-phase composites. For this, particles with polyhedral, undulated and other shapes were numerically modeled using analytical functions. Creation of some shapes, like polyhedral, are known from the literature [1] but Laplace's spherical harmonics [2], as well as the Goursat's surface and some others, were used for the first time to create novel particle shapes. Elastic properties of the composites with different particle shapes were calculated using the finite element analysis. The obtained results show good agreement with mean-field homogenization methods such like Mori-Tanaka and Lielens as well as other numerical results available in the literature [3]. Further, the dependence of the effective Young's moduli of the composite on the shape and the corresponding surface-to-volume ratio of the particles was studied.

For polyhedral, rotation symmetric and some other particles, the elastic properties of the composite were calculated and it was shown that for a particular volume fraction of the particles, an increase in the surface-to-volume ratio ψ results in an increase in the effective Young's modulus of the composite.

Comparing elastic properties, especially for the particles that are morphologically close to each other, e.g. particles obtained by Laplace harmonics, shows that the composites with these particles show dissimilar values of Young's moduli in spite of having the same surface-to-volume ratio. It can be concluded, that not only the surface-to-volume ratio but also other parameters like local surface curvature, concavity/convexity and sharpness of edges describing the local particle's geometry have substantial influence on the effective elastic properties of the composite. From this point of view, the studies of the correlation of these parameters with elastic properties of the particulate composites will be also interesting for the future studies.

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GENERATIVE AI DESIGN OF MULTI-MATERIAL ROTORS FOR HIGH-PERFORMANCE PROPULSION APPLICATIONS

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ABSTRACT

The turbine of oxidizer-rich turbopumps in reusable oxidizer-rich and full-flow staged combustion rocket engines. These systems subject blisks to rapid thermal transients (10^4 °C/s) on startup and shutdown which drive low cycle thermal fatigue; extreme centrifugal loads and high operating temperatures (>700 °C) which drive creep; and high-pressure, high-temperature oxygen rich environments which drive catastrophic metal fires (e.g., if the rotor rubs against a stationary component). Conventional blisks in oxidizer-rich turbines are solid components made from single materials; common material choices include cupronickel alloys, Haynes 214, and Incoloy 909 because of their burn resistance, strength, and thermal shock resistance, respectively. However, because of low cycle fatigue, creep, and inelastic yielding, the service life of conventional monolithic blisks is limited to ~10 flight cycles, far less than the 100s of flight cycles envisioned for next-generation reusable launch vehicles. Another issue complicating blisk design is that the high-strength Ni-superalloys most resistant to mechanical failure have high concentrations of reactive elements which make them susceptible to catastrophic metal fires, highlighting a design tradeoff between reusability and reliability. Multi-material blisks offer a potential solution to these problems. For example, a multi-material blisk could combine thermally stable alloys, high strength alloys, and a burn-resistant alloy case, leveraging the best features of each material to mitigate thermal fatigue, creep, and metal fires, thus unlocking previously inaccessible combinations of turbine inlet temperature, oxygen pressure, and shaft speed. Motivated by this concept, we have been developing an apparatus for rapid experimental assessment of key material properties and a complementary generative AI design tool which together can be used to discover optimal multi-material designs for thermostructural applications. This framework replaces the generation of traditional curated material property curves with active learning, employing AI/surrogacy tools over conventional process-structure-property relationships. I will describe how we are using this framework to design a continuum multi-material blisk system for an oxygen-rich turbopump operating at turbine inlet temperatures substantially higher with service lives an order of magnitude longer than current state-of-the-art monolithic blisks.

New trends in topology optimization
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OPTIMIZING ROTATING MACHINERY: A STUDY ON NATURAL FREQUENCY CONSTRAINTS APPLIED TO TOPOLOGY OPTIMIZATION OF FLUID-STRUCTURE INTERACTION PROBLEMS

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ABSTRACT

In some rotating machinery, the operation assembly presents tight tolerances, leading to wear problems caused by excessive vibrations. In this context, it is crucial to enhance the design of these components to reduce vibration levels and avoid resonant conditions. Based on that, this study focuses on topology optimization of fluid-structure problems considering turbulent swirl flow loading and natural frequency constraints on the 2D axisymmetric solids. The optimization problem proposed is compliance minimization subjected to volume and frequency constraints considering the three lowest natural frequencies. To ensure that the frequencies of interest are correctly constrained, the modal assurance criterion-based (MAC-based) mode-tracking method is employed to identify mode crossing during the optimization process. The governing equations are solved using separate domains, being the incompressible Reynolds-averaged Navier-Stokes equations with the k-ω turbulence model for the fluid, and linear elasticity with axisymmetry for the solid. The optimization method used is the Topology Optimization of Binary Structures with Geometry Trimming (TOBS-GT), which employs discrete (binary) design variables and different finite element analysis (FEA) and optimization meshes. Compliance sensitivities are computed through automatic differentiation using the adjoint method, while natural frequency sensitivities are derived through automatic differentiation using the forward method. Both FEA and sensitivities calculations are carried out in COMSOL Multiphysics. The integer optimization problem is solved via the branch-and-bound implementation in the CPLEX library. Three numerical examples are explored to study the design of the rotating solids through topology optimization. These examples include the rotating wall, the rotating and stationary wall system, and the stator structure. Results show that the method can increase the natural frequencies of the structures subjected to the interaction with a turbulent swirl flow in the context of rotating machinery.

Complex fluid flows in engineering: Modeling, simulation, and optimization
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CERTIFYING BIFURCATIONS IN ROMS VIA DEFLATED-GREEDY ALGORITHMS

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ABSTRACT

This presentation focuses on the development of tailored reduced-order models (ROMs) designed for bifurcating nonlinear parametric partial differential equations (PDEs). In this framework, multiple solutions can coexist for given physical/geometrical parametric values. Traditional certified reduced basis techniques struggle to accurately represent non-uniqueness phenomena, as error estimators become unreliable when bifurcations occur. Consequently, ROMs for bifurcating PDEs have always relied on compression strategies, such as proper orthogonal decomposition (POD), or machine learning data-driven approaches [1].

The main goal of the talk is to propose a novel greedy algorithm for bifurcating systems based on the deflation strategy, a technique capable of finding the coexisting solution branches simultaneously [2]. These algorithms can (i) certify multiple behaviors of the system with an efficient exploration of the parameter space and (ii) identify the parameter responsible for the non-uniqueness of the solution through an adaptive strategy.

The deflated-greedy method leverages several techniques, including deflation and continuation, to enrich the reduced space with bifurcating solutions. On the other hand, the adaptive-greedy approach exploits the non-differentiability of the solution as a function of the bifurcating parameter.
The effectiveness of these strategies is tested on a classical benchmark defined by the Navier-Stokes equations in a sudden-expansion channel, featuring a symmetry-breaking phenomenon with three coexisting solution branches. The results are compared in terms of accuracy and error certification against state-of-the-art methodologies, e.g. standard greedy and POD.

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Advances in computational biomechanics and mechanobiology
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE, MULTIMODAL COMPUTATIONAL MODELING OF MECHANOTRANSDUCTION IN THE DISTAL COLON AND RECTUM

Amirhossein Shokrani[1], *Bin Feng*[1] *and David Pierce**[1]

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ABSTRACT

Abdominal pain stemming from the large bowel is a primary manifestation of irritable bowel syndrome (IBS), significantly impacting quality of life. A major contributor to this pain is the mechanical distension of the distal colon and rectum. Mechanotransduction, the process converting mechanical stimuli in the colorectum into neural action potentials through sensory afferents, is pivotal in IBS-related bowel pain. Managing visceral pain in IBS remains a formidable clinical challenge due to the current limitations in research. While numerous medications effectively alleviate other types of pain, their efficacy in mitigating visceral pain is often limited, with potential adverse effects on the gastrointestinal system (GI). This study addresses this challenge by integrating experimental findings in afferent neural encoding and colorectal biomechanics into a comprehensive computational simulation framework. A three-layered, fiber-reinforced finite element model, accurately reproducing the nonlinear, heterogeneous, and anisotropic properties of the mouse colorectum using FEBio software, serves as the foundation. This model allows estimates of local mechanical stresses and strains around micron-scale afferent endings. The incorporation of a unique mechanosensitive neural membrane simulation replicates how local membrane tension encodes stress/strain into action potentials. Calibrated against experimental data, our neural membrane model considers NaV1.6 ion channels and mechanosensitive ion channels in spike initiation using NEURON. This multiscale model investigates three hypotheses on the mechanical gating of action-potential generation based on recent molecular-level insights into axon structure. Additionally, we explore the impact of afferent ending orientation on neural encoding properties. Beyond facilitating virtual analyses of colorectal mechanotransduction in prolonged visceral hypersensitivity, this work guides the design of new experimental studies to uncover the biomechanical and neurological mechanisms underpinning IBS-related bowel pain. Furthermore, it sheds light on potential mechanical and non-pharmacological interventions for colorectal diseases, contributing to the broader understanding and management of visceral pain associated with IBS.

FUZZY STATISTICS-AIDED INFERENCE IN EXPERIMENTAL DESIGN

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ABSTRACT

Classical approaches to the design of experiments (DOE) aim to minimize the number of experimental tests by strategically distributing test points in the controlled factor space related to the studied process. This is often coupled with imposing a specific form of predictive model, typically a low-degree polynomial. Uncertainty propagation analysis, accounting for measurement uncertainties and disturbances from uncontrolled factors, is traditionally conducted using classical statistics, assuming a normal distribution in most cases. The drawbacks of such an approach include significant inaccuracies in predictive models under more extensive ranges of controlled factor variability, disparities between actual and predicted distributions, and interpretational challenges due to excessive precision in statistics and risk assessments, which are essentially computational artifacts unrelated to physical reality.

Proposed solutions to overcome these challenges involve the application of fuzzy evaluations. Grzegorzewski [1] generalized the decomposition of the decision problem into three components in a decision-making context: the data set, the statistical hypothesis, and the requirements. Each of these elements can be considered separately as either fuzzy or non-fuzzy. Buckley [2] developed an extensive mathematical framework for fuzzy statistical hypotheses. Traneva, Atanassova, and Tranev [3] actively extended the applications of intuitionistic fuzzy sets to decision-making processes.

This paper compares classical DOE analysis and its extension, which uses fuzzy statistics and inference procedures. The studied process involves laser treatment of special coatings applied through electro-spark deposition (ESD), modifying the geometry of the surface layer to achieve desired tribological properties. The application of fuzzy modifications to the analytical and inference processes facilitated the interpretation of the obtained results. It also led to developing a data-driven predictive model, enabling effective forecasting of multimodal trends, which was not feasible with traditional quadratic models.

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Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INTERLAMINAR STRESS FORMULATION WITH EQUILIBRIUM BASED APPROACH APPLIED TO A SIMPLE MULTI-LAYER KIRCHHOFF-LOVE SHELL ELEMENT

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ABSTRACT

ABSTRACT

The present work focuses on equilibrium equations based on interlaminar stress formulation, applied to a new triangular multi-layer nonlinear shell finite element fully capable of simulating large displacements and rotations. The new shell element is an adaptation to a multilayer situation of the T6-3iKL element developed in [1], a Kirchhoff-Love shell kinematical model, considering the shell director across the layers as constant and the Rotation-continuity between adjacent elements and allowing multiple branches connections in the mesh. As a mean to guarantee the necessary degree of interpolation to represent the stress distribution throughout the thickness, the element considers strains along the edge of the element, as an extrapolation of the work developed in [2] and [3], and an additional bubble node. As for the interlaminar stress, an extremely simple approach is considered, a crank-nicolson equilibrium-based scheme, it is capable of representing complex stress distributions and establishing the foundations for future work on delamination analyses. The element is developed allowing for implementation of different material constitutive equations (Saint-Vennant, Neo-Hookean, and anisotropic materials). The model developed in this article is numerically implemented and results are compared to different references in multiple examples, showing the consistency and robustness of the formulation. It is believed that the multilayer extension with the desirable properties of no necessity of artificial penalty calibration, a simple kinematic, geometric exact, relatively small number of DOFs, the possibility to use 3D material constitutive models, easily connected with multiple branched shells and beams, and including possibly the simplest consideration of multilayers and interlaminar stress calculation, create a simple yet extremely capable shell element for interlaminar stress analysis.

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Advanced computational modelling of wood, wood-based products, bio-composites, and timber structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MULTI-PHYSICS FRAMEWORK TO INVESTIGATE THE COMPLEX FIRE-STRUCTURE INTERACTION IN MASS-TIMBER COMPARTMENTS

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ABSTRACT

The use of structural wood products, such as cross-laminated timber (CLT), has undergone a substantial increase in the construction of both mid-rise and high-rise buildings. This can be attributed to the appealing visual attributes it offers, as well as its fundamental focus on sustainability. Among, the different mass timber elements, CLT panels are massive wooden boards, manufactured by gluing timber planks with alternating grain directions (90°). The resulting panels possess structural, thermal, and acoustic properties, that make them fit for use in mid-rise and high-rise buildings. Despite these benefits, the mechanical properties of timber are affected when exposed to elevated temperatures such as those present in fire scenarios. In CLT slabs the fire exposed layer generally becomes charred and experiences a loss in strength, while the top side layer, heated during the process, sees a reduction in its load-bearing capacity. These combined effects could potentially lead to structural collapse. Therefore, to promote its widespread adoption, it is imperative to thoroughly comprehend, the structural, thermal and fire behaviour of timber structural elements. This study focuses on the structural performance of CLT slabs in closed compartments exposed to fire conditions.

To investigate the structural fire performance of CLT structures, a one way coupled Computational Fluid Dynamics (CFD) - Finite Element Method (FEM) numerical approach is used to model the complex fire-structure interaction. For the CFD fire analyses the software Fire Dynamic Simulator (FDS) is used, whereas the ANSYS is used for the transient thermo-mechanical simulations. For the coupling between the CFD and FEM models the Adiabatic Surface Temperature (AST) approach was adopted. In the CDF domain, the modelling of the entire compartment is carried out, including the geometry, thermal properties of the different materials and the input heat release rate representing the fire load. Then, the transient thermal and subsequent thermo-mechanical analyses of the CLT slab is carried out, yielding the temperature at different depths and the structural response. The influence of the charring wood on the exposed surface of the CLT slab is incorporated in two ways. First, the contribution of the charred wood to the ongoing fired is accounted for in the fire simulation model. Then, in the transient thermo-mechanical model the evolution of the damage charred layer is also incorporated. Finally, the model is employed to assess the thermo-mechanical and fire performance of CLT slabs exposed to fire in mass timber compartments.

Computational fluid dynamics (CFD) and fluid-structure interaction (CFSI): Methods and Applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RESOLVENT MODES AS THE FOUNDATION FOR LES WALL MODELS

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ABSTRACT

In Wall-Modelled Large-Eddy Simulations (WMLES) the flow away from a solid surface is resolved while the wall-layer is modelled. Typically, the interface between inner and outer layers does not coincide with the first grid point, and a buffer region is used to allow eddies to be created and develop into physically realistic structures. The present research aims to use Resolvent Analysis to synthesize near-wall eddies that are neglected in WMLES, thereby resulting in a more accurate representation of the momentum exchange between the bypassed near-wall layer and the outer flow. As a first step we calculate the force due to selected resolvent modes, and add it to the Navier-Stokes equations. The resolvent modes are characterized by their wavelengths in streamwise and spanwise directions, by their frequency and, very importantly, by the extent of their support in the wall-normal direction. Preliminary tests, carried out using a Wall-Resolved LES (WRLES), showed that (1) by changing the wavelengths of the resolvent modes we can affect independently various Reynolds stresses; (2) the resolved stresses adjust to the forcing, both in terms of their magnitude, and spectral distribution of the eddies responsible for the generation of shear stress $-\overline{u'v'}$; (3) that resolvent modes that span the inner/outer layer interface are more effective than those that lie entirely below this interface. Further tests consist of a series of WMLES in which the forcing due to various combinations of resolvent modes is added to the governing equations. Two Reynolds numbers are considered, Re=1,000 and 5,200. Since the resolvent modes were extracted from Re=1,000 calculations, the high-Re case provides a measure of how the approach can be extended to flow for which resolved LES or DNS data is not available. The use of the resolvent-mode-based forcing is found to affect the turbulent Kinetic Energy (TKE), which agrees better with the WRLES results. By selecting appropriate combinations of modes, the TKE and Reynolds-stress spectra are also improved, as the near-wall generation of eddies is enhanced by the forcing, in particular below the interface between outer and inner layer.

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Numerical approaches and discretization techniques for the geometrically nonlinear analysis of slender structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A KINEMATICALLY-EXACT REDUCED-ORDER ROD MODEL FOR ELASTOPLASTIC FAILURE IN THIN-WALLED MEMBERS

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ABSTRACT

This work profits from the embedded discontinuity FEM (ED-FEM) framework and a multiscale approach to derive a 7-DOF kinematically-exact reduced-order rod model for thin-walled members (starting from [1]) with a plastic hardening/softening constitutive equation (based on [2]-[3]) that emulates the coupling between local buckling effects and plasticity. The model is being implemented in an in-house finite element program for flexible thin structures, and shall be validated against reference solutions. The novelty as compared to [2]-[3] is the extension to the fully 3D context, including torsion-warping degrees-of-freedom and arbitrary (plastic) failure mode capabilities, allowing for the modelling of complex structural problems involving thin-walled members. Although kinematically-exact rod models are able to detect critical loads and represent post-critical configurations in most common scenarios, issues are bound to emerge when local effects (such as buckling of web and/or flanges) are relevant, especially when they are coupled with plastic deformations. For rod models, the combination of those factors can be satisfactorily represented in a phenomenological way by embedding them on a stress-resultant/cross-sectional strains hardening-softening plastic model, instead of enriching the model´s kinematics and related material law. One can employ multiscale modelling to generate constitutive relationships among the different strain and stress measures already containing information about plasticity, loss of geometrical stiffness, local buckling and even fracture conditions, with no or little increase on the number of degrees-of-freedom. The initial yielding behaviour can be handled through a plastic with hardening constitutive equation, whilst later buckling-plastic effects that lead to overall loss of bearing capacity of the structural element can be handled through a plastic with softening constitutive equation, in which discontinuities such as plastic hinges are present. For problems that involve strong discontinuities, the ED-FEM approach (see [2]-[3]) is an ideal match, allowing a local treatment of said discontinuities in a rather straightforward way. This approach introduces incompatible modes that have effects only inside the containing element, enriching its kinematics locally. Each incremental step of the numerical solution is solved by means of a split operator, whereby a Newton method´s step is performed with the usual rod´s DOFs (the local variables related to the discontinuities are statically condensed inside the elements), and then the local variables are solved in an element-wise fashion. This procedure adds little extra computational cost and proves to be quite robust, despite spoiling the quadratic convergence of the overall solution procedure.

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Computational particle-based solvers for multiphysics & multiscale simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN INTEGRATED EXPERIMENTAL APPROACH FOR EROSION DYNAMICS: TRANSIENT TO STEADY-STATE

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ABSTRACT

Transient erosion dynamics are characterised by rapid and often unpredictable changes in landscape, as dune erosion, due to short-term, intense events such as heavy rainfall, wind, flash floods, or human activities [1]. To capture these dynamics, our methodology integrates controlled laboratory experimental studies [2]. In the laboratory, experimental setups aim to replicate the effect of various erosion-inducing conditions, such as intense precipitation or concentrated flow. These controlled experiments enable precision control of erosion and deposition rates.

Steady-state erosion dynamics refer to the long-term, gradual processes of landscape alteration that occur under relatively stable environmental conditions. To study these dynamics, our approach integrates controlled laboratory experiments that simulate soil loss and permanent transects to accelerate laboratory data generation of representative erosion dynamics over extended periods in the field. These studies provide insights into the cumulative effects of erosion, factors influencing soil stability, and the effectiveness of erosion control measures.

An integrated approach for generating transient and steady-state erosion data provides a more holistic understanding of erosion processes. This experimental methodology not only helps in deciphering the immediate impacts of erosive events but also in understanding the long-term evolution of landscapes under continuous erosive forces. Such comprehensive data is essential for developing effective modelling strategies that can be used to predict soil conservation strategies, inform land-use planning, and mitigate erosion-related environmental impacts. By identifying appropriate model forms and calibrating erosion prediction models using the experimental data from transient and steady-state studies, we enhance the validity and applicability of the erosion prediction model. This integrated experimental approach application bas been faced up for a first application to coupled MLMs-DEM GPU (Meshless Lagrangian methods and Discrete Element Methods) models. Water-saturated system composed of particle bed that is immersed in a fluid has been simulated to obtain transient erosion with several particle size via MLMs-DEM simulations [3].

In summary, generating experimental validation data for erosion dynamics, encompassing both transient and steady-state aspects, is crucial for developing and refining erosion prediction models. This integrated approach is key to understanding and managing erosion processes in diverse environmental settings.

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Uncertainty quantification in structural dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADVANCES IN HIGH-PERFORMANCE STRUCTURAL DYNAMICS SIMULATION SOFTWARE TOWARD CHARACTERIZING STRUCTURES IN COMBINED ENVIRONMENTS

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ABSTRACT

Sierra Structural Dynamics (SD) is a massively parallel, finite element-based structural dynamics simulation tool developed at Sandia National Laboratories to conduct important simulations supporting broad national security missions. SD has historically seen use in a variety of mechanical engineering applications, including modal analysis, random vibrations, shock response, and transient combined environments analysis, such as coupled structural-acoustics, thermal-structural, and especially fluid-thermal-structural interaction.

The ever-evolving combined environments specifications from engineers necessitate advances in the software's physics capabilities, and the high-fidelity models needed to capture uncertain structural loads and other challenging physical phenomena also require new software developments to fully utilize our modern, heterogeneous high-performance computing platforms.

This talk will focus on recent efforts in SD, including physics enhancements to characterize complex and uncertain structural damping, as well as assessments of performance and scalability for combined environments simulations.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology \& Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Multi-scale, multi-rate damage and fracture: Models, experiments, and simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

QUASI-BRITTLE FRACTURE MODEL FOR BERYLLIUM

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ABSTRACT

Beryllium is a challenging and interesting material to model; it retains ductility even when it fractures and exhibits twinning as well. Its dynamic response is highly rate-dependent. In an attempt to capture its complex behavior, a model called QBrT has been proposed. It is a mechanism-based, continuum-level model that incorporates viscoelasticity, twinning, and brittle damage in both compressive and tensile state. It accounts for the material behavior in a wide range of strain, strain rate, and temperature. We have parameterized this model for Beryllium and validated it using the plate impact experiments. We will present the simulation results of the Richtmyer-Meshkov instability (RMI), and compare them with the experimental results and the simulation of RMI using a plasticity model PTW. In conclusion, QBrT-Beryllium outperforms the PTW. Using this example, we will discuss the necessity of the Uncertainty Quantification (UQ) in the materials modeling.

Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PRE-TRAINED TRANSFORMER MODEL AS A SURROGATE IN MULTISCALE COMPUTATIONAL HOMOGENIZATION FRAMEWORK FOR ELASTOPLASTIC COMPOSITES

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ABSTRACT

A composite material typically exhibits complex behavior at the engineer scale, arising from the interactions between its underlying constituent phases, as well as the competitions between micro-processes. It is generally a daunting task to develop an engineering model to adequately capture the essential micro mechanisms that propagate onto the macro scale. To this end, the multiscale computational homogenization method enables a consistent coupling across length scales, to give results that compare well with direct numerical simulations (DNS) having the full micro-structural details, without the need for any constitutive assumptions nor calibrations at the macro scale. Despite its predictive capabilities, the typical computational homogenization method is still computationally too expensive for most practical problems, as the coupling between micro and macro scales are solved simultaneously during its numerical implementation. In this presentation, focusing on the elastoplastic behavior of fiber-reinforced composite, we address this bottleneck with an offline development of a microscopic surrogate model for a given micro-structure, to be incorporated into a standard nonlinear FE framework, for rapid online implementations at the macro scale. For the offline training phase, we adopt the transformer-based architecture within a pre-training and fine-tuning framework. The proposed pre-trained transformer model is capable of parallelizing computations to effectively capture global dependencies within the strain-stress data sequences. To reduce the data generation cost, a constructed source representative volume element (RVE) having a single central heterogeneity with an identical volume fraction with the target RVE is utilized, to rapidly generate a huge source dataset for a pre-training process. The surrogate model is incorporated into a macro FE framework, and its predictive capabilities illustrated via the generic loading of two specimens with different microstructures, each having a different loading-unloading path.

Predictive digital twins
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREDICTING AND CONTROLLING SINTERING-RELATED DEFORMATION AND DISTORTION WITH SURROGATE MODEL AND DIGITAL TWIN

Peter Polak[*1], Ran He[1], Mingxuan Xia[1], Baber Saleem[1], Xiaoxia Yu[1] and Jingzhe Pan[1]*

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ABSTRACT

In ceramic manufacturing, controlling sintering-related deformations, including distortion, is of paramount importance. Finite Element Analysis with a well-suited constitutive law, can effectively predict sintering deformations and distortions. However, obtaining the necessary parameters for the constitutive law can be challenging. To address this issue, we employed an Artificial Neural Network (ANN) to establish a correlation between the parameters of the constitutive law and the corresponding predictions made by Finite Element Analysis, creating what we refer to as a Surrogate Model. This Surrogate Model is then used in a reverse manner within a Digital Twin framework to deduce the constitutive law's parameters based on observed sintering distortions during the manufacturing process.

Physics-informed machine learning for numerical modelling in engineering and science
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICS-INFORMED MACHINE-LEARNING SOLUTION OF NONLINEAR PARTIAL DIFFERENTIAL EQUATIONS USING THE KOLMOGOROV-ARNOLD REPRESENTATION

Mikhail Poluektov[1]*

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ABSTRACT

In 1950s, Andrei Kolmogorov and Vladimir Arnold showed that any continuous multivariate function can be represented by a specific composition of functions of a single variable [1]. Since then, it has been noticed that the Kolmogorov-Arnold (KA) representation can be a convenient machine-learning regression model – a predictive model that maps some vector input of a black-box system into a scalar output. However, the original Kolmogorov's proof was not constructive and did not provide insights into building the underlying functions of the representation based on the input-output data. There is a series of works that gives constructive proofs of the Kolmogorov's theorem and proposes convergent algorithms for determining the functions, see e.g. [2]. Recently, a lightweight iterative algorithm for construction of the underlying functions has been proposed [3] and subsequently improved (see arXiv preprint by the same authors), which simplifies the use of the KA representation as a machine-learning tool.
It has been shown that the KA representation in application to data modelling tasks performs equivalently to neural networks in terms of accuracy, but can require less computational time and resources for model identification, while having a capability to be implemented in a simpler code [3].
Physics-informed machine learning is an emerging field focusing on embedding physical constraints (e.g. conservation laws) into machine-learning models. One of the tasks considered within this field is solution of nonlinear partial differential equations (PDEs) using neural networks, which transpired to be a useful alternative to the established numerical discretisation schemes, especially in the case of scarcity of boundary data.
In the present talk, it is shown that the KA representation can also be used as a backbone of an efficient data-driven nonlinear PDE solver. The approach consists in replacing the unknown function of the PDE by the KA representation and identifying the parameters of the representation using the internal data generated by the PDE and the boundary data provided by the user. Several computational examples are given, including from the field of computational mechanics.
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Fracture, damage and failure mechanics of cementitious materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MESOSCALE MODELLING OF NEUTRON-IRRADIATED CONCRETE

Beatrice Pomaro[1], Jiangkun Zhang[1], Gianluca Mazzucco[1], Beaudin Freinrich Dongmo[1], Valentina Salomoni[1] and Carmelo Majorana[1]*

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ABSTRACT

In the context of ongoing license renewal and extended operation of in-service commercial nuclear power plants, there is an increasing focus on evaluating the long-term durability of concrete biological shields. To address this, a numerical approach is proposed within the framework of continuous computational methods. Specifically, a 3D thermo-mechanical and neutron diffusion (TMN) model for irradiated cementitious materials is developed, aligning with the Finite Element Method (FEM) at the mesoscale [1]. At this scale, the model accounts for radiation-induced volumetric expansion of aggregates as the primary interaction due to radiation. It incorporates a two-group neutron diffusion theory combined with heat conduction in the presence of thermal neutron capture.
Regarding the mechanical field, the model includes visco-elasto-plasticity and damage mechanisms [2], incorporating the most relevant interactions with radiation-induced material nonlinearities. A realistic geometry of a mesoscale concrete sample is numerically reproduced by treating it as a two-phase composite material consisting of aggregates and mortar. To validate the proposed model, an experimental study from the literature [3] is simulated. The numerical results in terms of damage propagation in neutron-irradiated concrete obtained with the model are juxtaposed to experimental results. This demonstrates the predictive capability of the proposed model for radiation damage triggering and evolution in concrete materials.

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Enabling technologies for digital twins: Model reduction and scientific machine learning
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTATIONAL MECHANICS AND SCIENTIFIC MACHINE LEARNING FOR DIGITAL TWINS IN CRITICAL INFRASTRUCTURE PROTECTION

Alexander Popp[12], Tarik Sahin[1], Jacopo Bonari[2] and Max von Danwitz[2]*

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ABSTRACT

The research field of computational mechanics, when interfaced with the advancements in scientific machine learning, opens new horizons in the development of digital twins, especially in the realm of critical infrastructure protection (CIP). This paper presents an integrated approach that combines traditional computational methods with novel machine learning techniques, thus aligning with the session theme "Enabling Technologies for Digital Twins: Model Reduction and Scientific Machine Learning".

Our initial focus delves into two foundational applications from our academic research at the University of the Bundeswehr Munich. The first encompasses the modeling and simulation of rough surface contact using traditional Boundary Element Methods (BEM). This established method is contrasted with our explorations in data-driven surrogate modeling techniques, showcasing how scientific machine learning can augment traditional computational mechanics. The second application transitions to the modeling and simulation of 2D and 3D contact mechanics. Here, conventional Finite Element Methods (FEM) are placed side by side with our recent work on Physics-Informed Neural Networks (PINNs).

The presentation then shifts its focus to address the emerging problem class of protecting critical infrastructures. At the DLR Institute for the Protection of Terrestrial Infrastructures, our group is spearheading the development of digital twins for this purpose. The primary goal is to forge accurate, reliable, and meaningful digital representations of critical infrastructure components for structural health monitoring, system surveillance, and the prediction of failure scenarios.

Among our ongoing projects, we spotlight a few key examples. The first involves the development of virtual sensing techniques for reinforced steel components in bridges, an initiative that merges model order reduction with computational mechanics. Another example details our efforts in simulating hazardous gas dispersion, utilizing model order reduction to enhance computational efficiency while maintaining accuracy. Lastly, we discuss our approach to damage assessment in critical infrastructures like wind turbine blades and bridges, employing physics-informed machine learning techniques to detect and predict structural weaknesses.

While the first part of this contribution presents mature and quantitative results from our academic research, the second part transitions to our current, more qualitative work-in-progress. This progression reflects the evolution from foundational research to applied, real-world challenges in critical infrastructure protection. Our work exemplifies the synergistic potential of computational mechanics and scientific machine learning, not just as discrete disciplines, but as integral components in the creation and implementation of digital twins for critical infrastructure protection.

Architected materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DESIGN AND MECHANICS OF 3D WOVEN ARCHITECTED MATERIALS

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ABSTRACT

Three-dimensional (3D) architected materials provide a pathway to defy the limitations of monolithic materials through their engineered internal microstructures, allowing them to exhibit unique and extreme properties. Thus far, research on the design of these architected materials has been primarily dominated by the quest to achieve extreme stiffness and strength, which limits their applicability in various fields. Unlike conventional truss-based architectures which induce stress concentrations and fail at strains lower than their constituent material, compliant woven architectures have recently been demonstrated to be able to sustain large tensile strains (several times larger than its constituent). However, the complex mechanics of woven architectures remain to be fully understood, and substantial bottlenecks exist in their design.

Here, we provide a computational design framework for woven architected materials that allows for spatial variation of fiber- and lattice-level parameters, allowing rapid generation of functionally graded architectures that can be fabricated at the micron scale and beyond. Variation of parameters at the sub-unit-cell level (on individual truss elements) greatly extends the design space and facilitates new modeling methods for these materials. Through reducing the lattice to a graph representation in order to create the weave topology, we facilitate the creation of woven architected materials with tailorable mechanical properties. Using this design framework, we present two modeling routes (high-fidelity and reducer-order) to quantify the architecture-dependent nonlinear properties, attributing contributions to nonlinear material properties and frictional contact. We discuss a specific hybrid design that attains improved stiffness and energy dissipation properties before failure. Through in situ micro-tension experiments to validate our models, we demonstrate that hybrid woven architectures can not only exhibit higher stiffness (more than an order of magnitude) than pure woven architectures, but also attain higher dissipated energy densities than the sum of their counterparts. This work aims to provide a pathway for the design of architected materials with tunable stiffness and enhanced toughness by harnessing deformation mechanisms in 3D woven architected materials. This fundamental mechanical understanding is useful for a wide range of applications, such as the development of 3D bio-scaffolds with engineered mechanobiological environments or soft pressure sensors with programmable electromechanical response.

EMBEDDED REDUCED MODELS IN THREE-DIMENSIONAL BODIES

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ABSTRACT

Problems in which the so called reduced dimensional models, such as beams, shells or membranes, are embedded into a solid domain arise in many engineering applications or physical modelling: reinforcement bars in concrete structures, fibers in composite materials or padle rackets are some examples. We present a complete theory for modelling reduced dimensional models embedded in deformable solids. Although there are several reduced dimensional theories, each one with its own different model, in this work we deal with a general type of these reduced dimensional models which encompasses the most typical ones for beams, shells, membranes… This common description allows us to generalise the strategy for the most common structure embedded in solid problems.

The presented theory works in both small and finite strain regime. Moreover, we complete it with a numerical discretisation strategy that yields convergent approximations. The ideas, based on the Arlequin method [1, 2], can be used to prove rigorously that the method is unconditionally stable for linear problems. Extending the same principles to the finite strain range we expect the resulting methods to perform well. Although no proof can be given in this case, the numerical results obtained confirm the robustness of the formulation.

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Uncertainty quantification and scientific machine learning for predictive modeling of complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TRUSTWORTHY AND SCALABLE DATA-DRIVEN CLOSURE MODELS

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ABSTRACT

Computational simulations of dynamical systems often require constitutive or closure models to represent unresolved phenomena, enhance computational efficiency, or correct model form error in the simulation. Data-driven closure models (DDCMs) employ machine learning (ML) to learn the closure term as a function of dynamic system states and have the potential to increase the predictive capability of computational simulations; however, trustworthiness and scalability of DDCMs are needed for adoption. In this work, we propose a methodology that addresses these needs by decoupling the estimation of the closure term from training the DDCM.

The time evolution of the closure term is estimated from experimental data using ensemble Kalman filters (EnKF) or other nonlinear filtering techniques. The DDCM is then trained independent from the dynamical system model, using the time evolution of the closure term as training data. Uncertainties that arise from sparse or noisy experimental data are mapped to the estimated closure term using the EnKF, then probabilistic ML algorithms propagate uncertainties to the DDCM. The approach is demonstrated on exemplar problems such as the Duffing oscillator, ecological models, and epidemiological models.

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Recent advances in partitioning method and interface mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL MODEL OF METAL-CERAMIC COMPOSITE WITH INTERPHASE PROPERTIES

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ABSTRACT

Multiphase metal matrix composites are used in modern industries like energy, aerospace, and automotive. The materials are used in severe loading conditions like impact loads or thermal shocks. The presentation concerns a data-driven model of an interpenetrated composite. The geometry of the material phases is obtained using CT scanning. Further details, namely, the distribution of voids and inclusions are found with the scanning as well. Based on CT scans the 3D finite element and peridynamics models are derived from. Former analyses [1, 2] showed the importance of the existence of an interface zone in multiphase composites. In the current presentation, the diffusion-based mechanism of forming the interphase zone is shown. A constitutive law evaluated in [3] is considered. The constitutive law for the cohesive zone was obtained using molecular dynamics simulations. The effects of the MD-based law on mesoscale samples are presented.

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Calculations: PL-GRID National Facilities: CYFRONET, Krakow, ICM at the University of Warsaw, TASK, Gdansk, Poland, and LUMI in Kajaani, Finland.

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Trustworthy multi-fidelity and data-driven models for computational applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NEURAL NETWORK APPROACH TO NUMERICAL APPROXIMATION OF INFINITY AND P-LAPLACE PROBLEMS

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ABSTRACT

Approximating solutions to infinity and p-Laplace problems poses numerical challenges, particularly for nonsmooth data. Infinity and p-Laplace equations appear in a variety of applications including image processing, optimal transport, and distance approximation. Numerical approximation via a finite element method is often effective but has some limitations such as large computation time on refined grids. We seek to examine the capabilities and accuracy of neural network solvers for infinity and p-Laplace problems. In this talk, we will present experiments using both physics informed neural networks (PINNS) and deep operator networks (DeepONets).

Biomechanics of hard tissues: From experiments and simulations to clinical applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A CARTESIAN-MESH STOCHASTIC FINITE ELEMENT SOLVER TO PREDICT BONE STRENGTH VARIATION

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ABSTRACT

Introduction
To bring a new drug to the market for bone disease, the effectiveness of the drug, i.e. improvement of bone strength, should be quantified by considering natural variability between individuals. A common practice to deal with bone variability is to apply a non-intrusive uncertainty quantification method such as Monte Carlo on finite element (FE) models of bones but with the drawback of requiring a large number of simulations. Here, a stochastic FE (sFE) solver was developed that uses an intrusive method to predict the variation in bone mechanics given the variability in bone tissue elastic properties.

Methods
The deterministic Cartesian-mesh (voxel-based) FE solver ParOSol [1] was used as the starting point. ParOSol solves the system of equations without storing the stiffness matrix, which leads to a very small memory footprint. The new sFE solver was developed by implementing the Polynomial chaos expansions (PCE) method [2]. The element-wise Young's moduli and nodal displacements were considered as uncertain inputs and outputs, respectively. The problem was solved using a conjugate gradients solver with Chebyshev's smoother preconditioning. PCE coefficients of nodal displacements were statistically analysed to quantify the variability in bone strength. The implementation was used to analyse an annular cylinder, a simplified diaphysis section (height, 0.03 m; inner/outer radii, 0.01/0.015 m), and meshed using hexahedral elements (1 mm). A deterministic and spatially homogeneous Poisson's ratio (0.3) was assumed. Young's modulus (10 GPa) was deterministic everywhere except in a 90˚ segmental region (height, 0.007 m) where it was spatially homogenous but normally distributed within the population (mean, 10 GPa; coefficient of variation 10%). The bottom face was held fixed, and the upper face was compressed by 10% of the height.

Results & Discussion
The propagated uncertainty through bone strength was quantified and compared with the corresponding result obtained by the converged Latin hypercube sampling of the Monte Carlo method, LHMC, with 2000 samples. The variance in bone strength obtained by the sFE solver has a 1.5% error compared with the one determined by LHMC. Moreover, the total computational time of the sFE approach was ~124x lower than LHMC.

Conclusion
The present evaluation demonstrates the correctness of implementation and provides an initial demonstration of the accuracy of the sFE solver.

Acknowledgements
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Architected materials and structures
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UNDERSTANDING THE MECHANICS OF RANDOM FIBER NETWORKS VIA NETWORK TOPOLOGY

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ABSTRACT

Architected materials exploit geometry to obtain novel mechanical properties and functionalities. A common strategy to engineer architected materials is to design a unit cell with desired properties, and then assemble these unit cells into a periodic array [1]. However, natural and biological systems often have aperiodic microstructure that leads to interesting emergent global mechanical behavior. Designing aperiodic structures is challenging because they can both correspond to a larger design space, and contain complex mappings between structure and mechanical properties. As such, there has been significant recent interest in understanding the interplay between geometry and the global mechanical behavior of materials for designing architected materials with aperiodic microstructures.

One class of metamaterials with aperiodic microstructure that is ubiquitous in biological and natural systems is random fiber networks. Compellingly, most random fiber networks in nature exhibit nonlinear strain-stiffening behavior under uniaxial tension. The strain-stiffening effect arises from fibers in the network transitioning from a softer bending dominated regime to a stiffer stretching dominated regime [2]. The strain-stiffening effect is also accompanied by the emergence of load paths in the fiber network, akin to force chains in granular systems [3]. However, the connection between force chains, fiber network kinematics, and the nonlinear mechanics of fiber networks are not well understood. In this work, we aim to link network topology and kinematics (structure) to the stress-strain response of discrete random fiber networks (function). First, we examine the mechanics of single fiber chains and relate the kinematics of these fiber chains to the mechanical response under loading. With the intuition from the mechanics of single fibers, we then look into the mechanics of random fiber networks. Specifically, we identified potential force chain candidates from the initial stress-free network structure and associated the emergence of these force chains to the strain-stiffening functional behavior of random fiber networks.

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New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION OF TIME DEPENDENT CONCENTRATED SOLID CHANNELS WITH INTERNAL HEAT GENERATION

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ABSTRACT

This work presents a novel topology optimization formulation for the Euler-Euler model applied to concentrated solid channels. Concentrated solids in fluid flow modeling are used in many relevant engineering areas, such as carbon capture and storage, electrochemical reactors, and fuel cells. One of these applications is a temperature swing adsorption (TSA) system. This system employs several stages to improve its efficiency. Inside these stages, adsorption takes place and generates heat. As adsorbent material temperature rises, its adsorption capacity decreases; thereby, temperature management is needed. Optimizing the topology of heat exchangers may reduce the operational cost and energy required for such a system. This investigation addresses fluid dynamics and thermal analysis, aiming to enhance the thermal efficiency of such systems by reducing thermal gradients and optimizing heat distribution within the channels. The forward problem is solved using a finite elements model, and sensitivities are obtained utilizing automatic derivation for the adjoint equations. The objective function is designed to minimize the internal energy inside the domain simultaneously. One example is presented to demonstrate the effectiveness and robustness of the proposed method. The example, an adsorption domain, demonstrates the formulation ability to handle time-dependent problems with internal heat generation. The results show that the optimized design can achieve significant improvements in performance over the initial designs, indicating the potential benefits of incorporating topology optimization and automatic differentiation into the design of systems based on Euler-Euler models. Additionally, results show that the design must be adjusted as solid density increases, which is relevant since most applications, such as fluidization, employ high-density solid materials.

Phase-field modeling: Analytics, benchmarks, and discussions
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHASE-FIELD METHOD AS APPROXIMATION OF THE SHARP INTERFACE THEORY WITH THE ORDER PARAMETER AS INTERNAL STATE VARIABLE

Andreas Prahs[*1], Daniel Schneider[12] and Britta Nestler[12]*

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ABSTRACT

The phase-field method is a well-established technique for simulating microstructure evolution in computational materials science [1]. It enables the numerically efficient tracking of material surfaces by means of an order parameter. The evolution equation of the order parameter is typically derived using a variational approach or by exploiting a corresponding principle of virtual power. In both cases, the order parameter is treated as an additional degree of freedom. In addition, both approaches consider a diffuse interface region from the outset. In this contribution, following the remark by [2], the order parameter is considered as an internal state variable instead of an additional degree of freedom. Moreover, the phase-field method is considered as approximation of the sharp interface theory of a continuum containing a singular surface [3]. The evolution equation for the order parameter is consistently derived within the framework of continuum thermodynamics through the exploitation of the Clausius-Duhem inequality. In this context, for the diffuse interface region, the heat conduction equation, the thermomechanical coupling, and the role of latent heat due to phase evolution are discussed. A comparison with the evolution equation obtained by the classical variational approach is carried out.

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Modeling, optimization and computational analysis of metamaterials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DYNAMIC CHARACTERIZATION OF ARCHITECTED METAMATERIALS USING REAL-TIME HYBRID SIMULATION

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ABSTRACT

Architected metamaterials are an emerging class of materials with extraordinary properties that can be tailored to achieve specific objectives by customizing their microstructural configurations. Further, the growth of additive manufacturing has enabled 3D printing of complex microstructures and has further stoked interest in this area. Applications areas of such architected metamaterials include mechanical, thermal, electrical, chemical, optical, magnetic and numerous others.

In this study, we focus on characterizing the dynamic performance of architected metamaterials such as energy absorption and wave attenuation under low velocity impact. We consider both, auxetic and nonauxetic microstructures, and study their response under plane wave propagation. A parametric study is conducted to evaluate how different microstructures perform and how their properties may be tailored to maximize wave attenuation.

A key objective of this study is to enable the use of real-time hybrid simulation (RTHS) for studying the dynamic characteristics of architected materials. With RTHS, that part of the metamaterial domain that is subjected to impact and undergoes large deformations and damage is modelled physically and other parts of the domain that remain linear are modeled numerically. A single actuator transfer system is used to connect the physical and numerical subdomains using an in-house Linux-based real-time execution platform. This effort is ongoing and challenges with conducting such RTHS and lessons learned will be presented.

REDUCED ORDER MODELING OF INCOMPRESSIBLE FLOWS

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ABSTRACT

Advancements in computational hardware and physical simulation techniques have pushed the envelope of complexity of scientific applications that can be modeled with adequate accuracy. However, these high-fidelity simulations of many challenging applications are expensive for multi-query applications, real-time simulation and dynamics forecasting. In such situations, reduced order models (ROMs) are an attractive alternative as they can simulate engineering systems at a lower computational overhead without a significant loss in accuracy. Projection-based ROMs rely on offline-online model decomposition, where the data-based energetic spatial basis is used in the expensive offline stage to obtain equations of reduced states that evolve in time during the inexpensive online stage.

The online stage requires a numerical scheme for the dynamic evolution of the coupled system of pressure and velocity states for incompressible fluid flows. Furthermore, the dynamic evolution of a large number of these reduced states in the online stage can be expensive. In contrast, the accuracy significantly decreases if only a few reduced states are considered and the interactions of the unresolved states with the resolved states are not accounted for. Ideally, ROMs should be consistent with the underlying full order model, which requires an appropriate strategy for the construction of operators. In this talk, we will present advancements in three areas of ROMs for incompressible flows: 1) solution method for the coupled continuity and momentum equation, 2) appropriate closure modeling for interactions between unresolved and resolved states, and 3) maintaining consistency between ROM and corresponding full order model. For the last area, we will discuss the trade-off between consistency and intrusiveness for continuous, discrete and data-driven approaches for constructing ROM operators.

Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ANALYSIS OF ENERGY DISSIPATION IN PARTICLE DAMPERS VIA THE DISCRETE ELEMENT METHOD EMPLOYING THE COMPLEX POWER METHOD

Braj Bhushan Prasad[*1], Tommy Luft[1], André Katterfeld[1], Elmar Woschke[1] and Hermann Rottengruber[1]*

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ABSTRACT

A particle damper is a passive damping system, which relies on the high dissipation properties of granular materials. The particle dampers can be mounted on the structure or can be inserted in existing cavities of the vibrating structure often without causing significant changes in the mass or stiffness of the original structure. The collisions of the particles with each other and with the cavity walls lead to friction-based dissipation and result in a reduction of the vibration amplitude of the carrying structure. The particle damping mechanism is highly non-linear and depends on several parameters, such as particle size, the number of particles, particle materials, and particle packing ratio, which restrict its real-world application. This contribution aims to present preliminary work in the development of models for assessing the damping characteristics of particle dampers utilizing the complex power method, which enables the analysis of energy dissipation in particle dampers without the need for an underlying vibrating structure. In general, the complex power is connected to a harmonic excitation cycle, and its computation involves using the velocity of the particle container and the force driving its excitation. The numerical investigation of the energy dissipation mechanism in particle dampers is conducted through the discrete element method (DEM) using the open-source code LIGGGHTS. This study employs a particle damper consisting of steel balls, chosen with the objective to expediting the calibration process, facilitated by the availability of material characteristics for steel balls in a data handbook. The methodology proposed in this study will undergo validation through an experimental investigation.

Innovations in machine learning-enhanced uncertainty quantification for computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

UNCERTAINTY REDUCTION WITH MULTI-MODEL MONTE CARLO FOR CRYSTAL PLASTICITY SIMULATIONS OF ADDITIVELY MANUFACTURED METALS

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ABSTRACT

In this work, multi-model Monte Carlo estimators are developed to reduce uncertainty in quantities of interest (QoIs) extracted from crystal plasticity simulations of additively manufactured (AM) metals. A significant concern in AM parts is uncertainty in mechanical properties caused in part by complex microstructures that arise from the AM process. Quantifying uncertainty in microstructure-sensitive behavior using experiments alone is costly, especially when mechanical allowables must be established. Quantitative relationships among microstructure, micromechanical metrics like slip accumulation, crack initiation, and failure are also difficult to capture with limited experiments. Crystal plasticity material models instead enable computational prediction of micromechanical stress and strain fields given a discretized microstructure. However, high-fidelity finely discretized crystal plasticity simulations are computationally expensive, while lower-fidelity models are less accurate and generally biased, making uncertainty quantification and reduction computationally difficult as well.

Multi-model Monte Carlo methods leverage correlations between high- and low-fidelity models to produce unbiased estimators for QoIs with reduced uncertainty relative to standard Monte Carlo. Crystal plasticity QoIs considered in this work include yield strength and the mean and extreme values of micromechanical fields that are relevant to crack initiation. Multi-model Monte Carlo estimators are developed for each individual QoI and several groups of QoIs. The results of this work establish relationships among model correlations, sample allocation, and uncertainty reduction for different combinations of QoIs and demonstrate a trend of less uncertainty reduction as QoIs become more sensitive to local microstructure. Limitations from using pilot samples to estimate model covariances and train low-fidelity models are also addressed. The uncertainty reduction achieved by multi-model Monte Carlo is an important step toward using computational mechanics models to predict microstructure-sensitive crack initiation and failure in AM parts.

A PROBABILISTIC GRAPHICAL MODEL APPROACH TO DECOUPLE MULTI-PHYSICS SYSTEMS

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ABSTRACT

Complex multi-physics systems, like those used in weather prediction and spacecraft simulation, often require coupling of subdomain models. However, this coupling is expensive - due to feedback, heavy communication overhead, and the need to ensure the delicate consistency of scenario parameters across domains. With the increased cost of running the model, downstream tasks like model calibration and uncertainty quantification can also become impractical. Thus, modelers aim to decouple these models as much as possible, while maintaining high accuracy in the model predictions. In this work, we demonstrate a method to decouple multi-physics models by learning an undirected graphical model corresponding to the system state variables. The edges in the learned graph represent conditional dependence between variables, which indicates the need for coupling between two models. This approach leverages information in available data - from either the real system or a high-fidelity model - to identify the most important couplings, and those which may be safely neglected.

Modeling and simulation of advanced manufacturing processes for metals
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOWARDS THE EXAMINATION OF PROCESS-PROPERTY RELATIONSHIPS OF WIRE ARC DED VIA THERMO-MECHANICAL FE SIMULATIONS

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ABSTRACT

The as-built internal residual stresses and part-level distortions from the wire arc DED process are highly dependent on machine process parameters and tool path. While multiple experiments are commonly performed for process parameter optimization, these experiments are typically limited in part volume and thus do not provide much information related to residual stresses or distortion. Additionally, the build up of multiple part replicates of sufficient volume for such an examination would be labor and cost intensive. Therefore, this work seeks to examine the process-property relationships of wire arc DED via thermo-mechanical FE simulations. Abaqus/standard with a moving heat source and material deposition are used to mimic the wire arc DED process. This work introduces modeling the substrate fixturing in addition to component being additively manufactured. Multiple variables of the printing process (e.g., process parameters, inter-layer dwell time, tool path) and as-built component (e.g., residual stresses, distortion) are studied. Additionally, material model fidelity is examined to determine the relative role of the material model on the mechanical predictions. The thermo-mechanical FE simulation results are compared with experimental data for model calibration/validation purposes. Preliminary results indicate a significant role of inter-layer dwell time on the as-built component's residual stresses and modeling the substrate fixturing leads to significantly different thermal responses in early layer printing of components.

GEOMETRIC MULTIGRID METHODS FOR A MATRIX-FREE STABILIZED SOLVER FOR THE INCOMPRESSIBLE NAVIER-STOKES EQUATIONS

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ABSTRACT

The fully-coupled finite element discretization of the incompressible Navier-Stokes equations requires the solution of a sequence of linear systems of equations that are saddle-point problems difficult to solve with traditional iterative methods. Geometric multigrid methods can be used as monolithic preconditioners for the linearized system if a stabilized finite element discretization is used. In this study, we compare two variants of geometric multigrid preconditioners, local smoothing and global coarsening, within a matrix-free solver [1, 2]. The multigrid variants are implemented in Lethe, an open-source computational fluid dynamics (CFD) software, which uses the deal.II finite element library and a continuous Galerkin discretization with SUPG/PSPG stabilization [3]. Multigrid levels are defined using the mesh hierarchy obtained by the refinement of the original mesh. While the global coarsening approach considers the entire domain for each level, the local smoothing approach uses only the most refined cells at each stage of the mesh refinement. This leads to different multigrid hierarchies when adaptive mesh refinement (AMR) is used. We compare the results of two benchmarks that benefit from AMR: the flow around a sphere and the backward-facing step, using different Reynolds numbers and equal-order velocity-pressure discretizations. The comparison is made in terms of iterations and parallel performance, using both strong and weak scaling. Preliminary results indicate that the global coarsening algorithm shows better parallel scalability than the local smoothing algorithm. Moreover, this study demonstrates that geometric multigrid preconditioners are promising for strongly nonlinear coupled problems and matrix-free implementations.

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Computational methods in environmental fluid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FINITE ELEMENT TECHNIQUES FOR MODELING HURRICANE STORM SURGE

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ABSTRACT

Storm surge due to hurricanes and tropical storms can result in significant loss of life, property damage, and long-term damage to coastal ecosystems and landscapes. Computer modeling of storm surge can be used for two primary purposes: forecasting of surge as storms approach land for emergency planning and evacuation of coastal populations, and hindcasting of storms for determining risk, development of mitigation strategies, coastal restoration and sustainability.

Storm surge is modeled using the depth-averaged shallow water equations coupled with wind forcing. Tides, riverine forcing, atmospheric pressure, bottom friction, the Coriolis effect and wind stress are all important for characterizing the inundation due to surge. The problem is inherently multi-scale, both in space and time. To model these problems accurately requires significant investments in acquiring high-fidelity input, accurate discretization of the computational domain using unstructured finite element meshes, and numerical methods capable of capturing highly advective flows, wetting and drying, and multi-scale features of the solution.

The combined effects of continuous and discontinuous Galerkin finite element methods allows for many of the features necessary to accurately capture storm surge physics. We describe the application of the computational techniques to hurricane storm surge.

Smart structures – Modelling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SELF-DIAGNOSIS OF ADAPTIVE STRUCTURES BASED ON THE REDUNDANCY CONCEPT

Tamara Prokosch[*1], Jonas Stiefelmaier[1], Christina Tarín[2] and Manfred Bischoff[1]*

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ABSTRACT

Sustainability calls for new technologies and saving resources. Due to the huge impact on global resource consumption, energy demand and waste production, adaptive civil structures might contribute to the answer to this calling. By incorporating sensors, actuators, and a control unit into the design of civil structures, active shape changes and stress redistribution become possible. This way, the structure can react efficiently to typically high, varying loads. Embodied energy in the high masses of bridges and high-rises can be purposefully used or reduced. However, as with any new technology, safety considerations are important, particularly when it comes to structural failure. The sensors and actuators in adaptive structures offer a unique opportunity, not only to monitor structural health and detect potential failure at an early stage but also to actively test the structure for damage. This allows for timely repair and support measures as well as a sustainable and long service life.

The first challenge for structural analysis lies in modeling the actuation and developing analysis methods with fundamental insight and high applicability. The redundancy matrix as such has been of particular importance for adaptive structures. By quantifying the constraint on each element exerted by the surrounding structure, the redundancy matrix provides insight into the response of the structure to actuation, modeled as an imposed actuator stroke. Gade et al. [1] proposed a generic matrix formulation for efficiently updating the redundancy matrix with application to truss and frame structures. This lays the foundation for investigations on the detection of structural failure of elements and changes in element properties due to changes in the redundancy distribution.

We conducted studies on various systems with different topologies and materials and implemented the redundancy distribution both for the original systems, as well as for variants with missing or damaged elements. Aiming for detectability measures, we analyzed changes in stress distribution and deformations for general load cases and changes in the redundancy distribution of the system. To validate the resulting measures, we implemented the model-based fault diagnoses for an adaptive high-rise structure and tested the efficiency.

This work is conducted in the framework of the Collaborative Research Centre 1244 funded by the Deutsche Forschungsgemeinschaft (DFG - German Research Foundation). The authors are grateful for the generous support.

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Advances in neural operators for scientific modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GRAPH NEURAL OPERATORS FOR QUANTIFICATION OF GEOMETRIC UNCERTAINTY

Adrienne Propp[*1], Amanda Howard[2], Mauro Perego[3], Alexander Heinlein[4], Daniel Tartakovsky[1] and Panos Stinis[2]*

[1]*Stanford University*
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[4]*Delft University of Technology*

ABSTRACT

We propose a graph neural operator that enables efficient uncertainty quantification for macroscale quantities of interest due to changing geometries. Our graph-based framework, in contrast to typical mesh-based approaches to PDE modeling, addresses the challenges of uncertainty quantification on random domains and alleviates the mesh dependency of many alternative methods. We will present the application of our method for ice-sheet dynamics that enables efficient quantification of the uncertainty related to glacial mass loss and allows for increased flexibility based on the ice sheet geometry, grounding line, and basal friction.

Methods for identification, machine learning, and uncertainty quantification of reduced order models of coupled systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MARKOV CHAIN MONTE CARLO CAPABILITIES IN DAKOTA

Ernesto Prudencio[*1] and Adam Stephens*[1]

[1]*Sandia National Laboratories*

ABSTRACT

This talk will be divided in four parts. We will first go through an overview of the different Markov chain Monte Carlo (MCMC) algorithms and companion Bayesian analysis functionalities that Dakota provides by interfacing itself with different external packages, such as the MIT Uncertainty Quantification (MUQ) and the Quantification of Uncertainty for Estimation, Simulation, and Optimization (QUESO) libraries. In the second part, we will have a more detailed exposition on the methods most recently added to Dakota through MUQ: the Metropolis adjusted Langevin algorithm (MALA) and the likelihood informed subspace (LIS) methods. The third part will present a comparison of the application of some MCMC algorithms to a set of problems, highlighting pros and cons of the different algorithms being compared. We will finalize the talk with a presentation of potential directions we might take in the future regarding (i) the improvement of current MCMC methods already available in Dakota, (ii) the addition of new methods, and (iii) the use of python to access MCMC capabilities in Dakota.

Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SOME OF PROFESSOR ODEN'S INVESTIGATIONS ON MODEL VALIDATION AND BAYESIAN ANALYSIS OF COMPLEX ENGINEERING AND SCIENTIFIC MODELS

Ernesto Prudencio[*1]*

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ABSTRACT

In this talk I will present some of the investigations I had the pleasure to conduct in collaboration with Professor Oden and other colleagues at The Oden Institute for Computational Engineering & Sciences at the University of Texas at Austin. More specifically, I will briefly talk about three different efforts: one in material damage control, one in nonlinear elatostatics, and one in tumor growth. Just this small sample of Professor Oden's work already gives us a glimpse on the breadth and depth of his investigative mind. These three different efforts cover areas such as uncertainty quantification, model calibration, model validation, model ranking, information gain analysis, optimal experimental design, and filtering.

E. E. Prudencio, P. T. Bauman, D. Faghihi, K. Ravi-Chandar, and J. T. Oden, A Computational Framework for dynamic data-driven material damage control, based on Bayesian inference and model selection, International Journal for Numerical Methods in Engineering, 102: 379-403, 2015.

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16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics

July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VERIFICATION AND VALIDATION IN COMPUTATIONAL MECHANICS

*Serge Prudhomme**[1]

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ABSTRACT

Verification and Validation are essential activities for predictive modeling in computational sciences and engineering. I will briefly describe some recent progress on related topics, for example, the verification of neural network approximations of solutions to boundary-value problems, the optimal design of experiments for validation of mathematical models, or a goal-oriented formulation for model calibration. More specifically, I will present a multi-level neural network approach capable of reducing the approximation error to machine precision. The method consists in estimating a correction in a previously computed neural network approximation by solving the problem for the residual error using a new network of increasing complexity. I will also describe a novel methodology to design an optimal validation scenario to assess the predictivity of a model in the cases where experimental data at the prediction scenario are unavailable and the quantity of interest cannot be observed. The method relies on solving two optimal design problems that best match sensitivity indices that one would obtain at the prediction scenario. Finally, I will present a novel approach for model calibration that simultaneously identifies the model parameters and the modeling errors. The novelty of the proposed calibration method lies in the fact that the values of the model parameters are now inferred with respect to the intended use of the model, which is expressed in terms of a given quantity of interest.

NONLINEAR MODEL ORDER REDUCTION WITH SMOOTH NEURAL FIELDS

Vedant Puri[1], Aviral Prakash[1], Jessica Zhang[1] and Levent Burak Kara[1]*

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ABSTRACT

There has been heightened interest in model order reduction for predictive modeling in light of recent advances in machine learning (ML). Reduced order models (ROMs) follow a separation of variables approach. First a reduced state representation is learned from data. Then, the reduced state vector is evolved in time following the physics of the problem. ML-ROMs, which apply nonlinear transformations to obtain powerful ROM representations, have been shown to outperform projection-based PCA-ROMs in advection-dominated fluid-flow problems [1, 2]. ML-ROMs, however, incur limitations as they are trained using autoencoders that learn to map high-dimensional simulation data from fixed grids to a reduced space [1, 2, 3].

In this work, we cut the training time in the offline stage by half by employing an encoder-less training approach where a decoder is learned along with reduced representations corresponding to trajectories in the training set. The decoder, a continuous neural field model, then learns a mapping from the reduced space to the space of continuous vector fields in a discretization-invariant manner [3]. Our model is therefore able to learn ROMs from simulations on adaptive and evolving grids where interpolation to a fixed mesh may be infeasible.

Once a reduced representation is learned, the problem is time-evolved per the governing PDE system, which involves computing spatial derivatives of the solution field. Prior works suffer from nonsmooth neural representations whose derivatives are corrupted by noise, and resort to low-order finite differencing on a supplementary coarse mesh [3]. We sidestep this problem by developing methods to learn smooth neural representations that can be differentiated exactly with automatic differentiation. Our key observation behind this improvement is that smooth neural representations can be learned by applying regularization to the decoder model during the offline training process.

In this presentation, we discuss our contributions which lead to faster offline-stage, and improved accuracy, performance during the online-stage. We demonstrate the efficacy of our methods on several 1D and 2D advection dominated traveling shock problems.

[1] Lee K et. al. Journal of Computational Physics 404 (2020) 108973.
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Multi-scale modeling and upscaling for flow induced vibrations, from local reference simulations to certified industrial tools
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ANALYTICAL FRAMEWORK AND NUMERICAL VALIDATION FOR FLUID-STRUCTURE INTERACTION OF FLEXIBLE COAXIAL CYLINDERS

Maria Adela Puscas[1] and Romain Lagrange*[1]

[1]*CEA, DES, ISAS*

ABSTRACT

This study delves into the analysis of small-amplitude forced beam vibrations of two coaxial finite-length cylinders separated by a viscous Newtonian fluid. To tackle this complex phenomenon, we introduce a novel theoretical approach rooted in the Helmholtz expansion of the fluid velocity vector. This method enables us to derive a comprehensive analytical expression for the fluid forces, subsequently providing insight into the modal added mass and damping coefficients [1].
Our theoretical framework reveals a noteworthy finding: the fluid forces exhibit linearity with respect to the Fourier harmonics of the vibration modes. Importantly, the coefficients governing these linear combinations are found to be contingent upon the aspect ratio of the cylinders, the separation distance, and the Stokes number. Consequently, the linear fluid forces do not invariably mirror the shape of the forced vibration mode. Instead, the fluid introduces the intriguing possibility of coupling vibration modes with distinct wave-numbers.

In contrast to prior research efforts, our current theory surpasses limitations by incorporating viscous effects of the fluid, accounting for the finite length of the cylinders, avoiding reliance on the assumption of a narrow annulus, and encompassing all classical boundary conditions for an Euler-Bernoulli beam within a unified formulation.

To validate our theoretical predictions, we conduct numerical simulations (TrioCFD [2] open source code with an ALE module) considering various boundary conditions such as rigid, pinned-pinned, and clamped-free vibrations. The results not only support the proposed theoretical framework but also shed light on the nuanced interplay between fluid dynamics and structural vibrations under diverse boundary conditions. This comprehensive approach advances the understanding of forced vibrations in complex systems involving fluid-structure interactions.

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Contact and interface mechanics: Modeling and computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ON A STRUCTURE PRESERVING IMPLICIT DYNAMICS CONTACT ALGORITHM.

Michael Puso[1] and Cosmin Petra*[1]

[1]*Lawrence Livermore National Laboratory*

ABSTRACT

A newly developed contact algorithm [1] that exactly conserves discrete energy and momentum has been developed. In addition, the new approach avoids the chatter typically encountered with most contact algorithms during persistent contact. Standard time integration schemes such as Newmark's method are well known to have stability issues and chatter in the event of unilateral contact. This is due to inherent smoothness built into these time integration schemes and the lack of control of the energy due to the nonlinear nature of the impact. A large body of literature has been devoted to treat these inherent issues of implicit contact but few if any conserve a discrete form of energy and momentum, eliminate chatter whilst enforcing both gap and velocity constraints by way of Lagrange multiplier. This is accomplished here by developing a new mortar projection scheme that conserves angular momentum by construction The chatter is eliminated by modifying the midstep time integration such that the updated velocity satisfies a biliteral gap velocity constraint. The discrete energy of the contact is conserved by employing a time integrated algorithmic gap. The gap calculation is exact in 1D, doesn't drift and the error can be bounded by the time step. Examples that demonstrate the robust character, accuracy and unbiased contact are demonstrated.

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Modeling, simulation, and AI for ultrasonic NDT and SHM
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NON-DESTRUCTIVE STRESS WAVE AMPLITUDE TESTING FOR INTERFACE BONDING STRENGTH OF 3D PRINTABLE CONCRETE

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ABSTRACT

This study aims to explore the impact of interface bonding properties of the concrete on non-destructive testing. Various concrete samples with different numbers of layers and time intervals were printed. Non-destructive testing was conducted using an ultrasonic device. Because of the presence of interface layers, 3D printable concrete exhibits slower wave propagation velocity and smaller wave amplitude than casted concrete. Moreover, the amplitude considerably increased while the number of printing layers and intervals increased. The amplitude attenuation could be attributed to losses caused by stress wave transmission between the transducer and the test piece. It was also resulted from the height of the concrete, as well as the printed interface layer. It shown a linear relationship with the interface bonding strength of the cement-based material. The interface bonding performance of 3D printable concrete was investigated through the observed pattern of amplitude attenuation using the non-destructive testing approach. It is demonstrated that the interface bonding properties exhibit anisotropic mechanical performance resulted from the layer-by-layer additive printing technique employed in 3D printable concrete. In comparison to casted concrete, the interface layer in 3D printable concrete considerably affected the transmission of stress waves. It could be a fundamental factor resulted in differences in non-destructive testing.

Recent advances in computational fracture mechanics and failure analysis
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN IMPROVED HYBRID COMPUTATIONAL MECHANICS FRAMEWORK FOR COMPOSITE DAMAGE MODELLING AND SIMULATION

Heng Liu[12], Gang Qi[1], Il Yong Kim[2] and Diane Wowk[3]*

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ABSTRACT

Fiber-reinforced polymer composite systems have been replacing traditional metallic materials at an unprecedented rate for airframe structures, driven by the essential needs for lightweight and improved structural performance to achieve high demands on aircraft sustainability objectives. Meanwhile, damage tolerance assessment of composite structures presents significant difficulties for airworthiness certification and aircraft sustainment due to their complex damage and failure mechanisms. Although considerable research has been devoted over the past decades to developing high-fidelity composite damage computational models, having the capability to effectively and efficiently predict complex composite damage and failure behavior is still a daunting challenge. All existing modelling strategies for composite damage evolution suffer from either inaccuracy, modelling cumbersomeness, or formidable computational cost. This study aims to develop an improved hybrid computational mechanics framework to capture the major failure modes of each composite ply and predict their progressive damage evolution in a composite laminate. An integrated modelling approach is proposed, combining continuum damage modelling (CDM), the extended finite element method (X-FEM), and the cohesive zone modeling (CZM) technique, to capture fiber fracture, matrix cracking, and interlaminar delamination. The Schapery theory (to address polymer matrix viscoelastic behavior) is incorporated with the 3-D Hashin failure criteria to accurately simulate the pre-peak nonlinearity of the load-bearing response due to matrix microcracking. The proposed hybrid model is developed and implemented using Abaqus with user-defined subroutines. Multidirectional composite laminates with open-hole notch configurations under tension (OHT) and compression (OHC) loading scenarios are examined. The simulation results are compared with the physical experiments and numerical models in the open literature and demonstrate the effectivity and practicability of the modelling methodology for composite progressive damage analysis. In conclusion, such a modelling and simulation methodology shows a noticeable improvement in composite damage modelling. It represents a practical paradigm, which not only drastically reduces the pre-processing workload to build a physics-based high-fidelity damage model, but also largely decreases the computational cost.

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Computational methods for wind energy
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREDICTING FAR WAKE INTERACTION IN WIND FARM BY HIGH RESOLUTION 2D LES SIMULATION WITH POROUS DISK MODEL

Ji Qi[1], Kenji Ono[1], Koichiro Shibuya[1] and Takanori Uchida[1]*

[1]*Kyushu University*

ABSTRACT

Numerical fluid dynamics has become an essential tool in wind turbine design, and recent large-scale simulations using LES models have provided highly detailed information. In the design of large offshore wind farms, accurately simulating the interaction of wake flows behind wind turbines is crucial for predicting the overall power generation performance of the wind farm. However, conducting LES simulations on such a large scale across the entire wind farm requires impractical huge computational resources, even when using state-of-the-art supercomputers. To mitigate computational costs, various surrogate models such as Actuator Line Model / Actuator Disk Model and light-weight engineering models for approximating wake flows have been employed. We have proposed a simple porous disk model as a surrogate model and confirmed its excellent reproducibility in replicating the mainstream velocity distribution when compared to actual measurement data [1,2]. The advantage of the porous disk model lies in its ability to be implemented in two dimensions, distinguishing it from other surrogate models. Therefore, by implementing the porous disk model into a 2D LES code and conducting high-resolution simulations, we were able to simulate interference scenarios of wake flows from multiple wind turbines that cannot be replicated by engineering models, enabling us to perform unsteady wind condition analysis for the entire wind farm. The code is capable of efficient computations through parallel processing using OpenMP/OpenACC. In this presentation, we will demonstrate not only showcase a comparison between the results of 2D LES simulations and experimental data but also provide insights into comparisons with engineering models, computational time considerations, and the characteristics of wake flow interactions.

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Data-driven approaches for solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A FRAMEWORK OF CONVOLUTIONAL HIERARCHICAL DEEP NEURAL NETWORK FOR NONLINEAR FINITE ELEMENT AND MESHFREE ANALYSIS

Yingjian Liu[1], Jiachen Guo[2], Chanwook Park[2], Wing Kam Liu[2] and Dong Qian[*1]*

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[2]Northwestern University

ABSTRACT

In this presentation, we introduce a framework for the Convolutional Hierarchical Deep Neural Network (C-HiDeNN) designed for nonlinear finite element and meshfree analysis. Building upon the structured foundation of HiDeNN [1], which encompasses the evaluation of shape function derivatives, adaptivity, and material derivatives [2], C-HiDeNN [3] incorporates a convolution operator to enhance the HiDeNN approximation. The distinctive feature of C-HiDeNN lies in its provision of an expanded set of optimization parameters, including the polynomial basis number 'p,' dilation parameter 'a,' patch size 's,' and mesh position 'x.' These parameters serve as the weights and bias parameters of the C-HiDeNN patch. To underscore the effectiveness of this framework, we present numerical examples within the context of nonlinear finite element and meshfree analysis. The results demonstrate that our approach achieves significantly higher accuracy compared to the regular Finite Element Method (FEM) with a substantially reduced computational cost.

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Catastrophic failure mechanics and numerical modelling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GENERALIZED STRENGTH REDUCTION METHOD FOR DETERMINING THE FACTOR OF SAFETY OF CONCRETE STRUCTURES

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ABSTRACT

The strength reduction method (SRM) was originally used in a slope stability analysis, and it was applied by reducing the shear strength of geomaterial. However, in case of concrete, damage occurs due to not only exceeding the shear strength, but also exceeding the tensile strength or compressive strength, SRM should be modified and adapted to concrete strength criterion. The paper presents a modified SRM for determining the factor of safety (FoS) of concrete structures with multi-parameters strength criterion. Instead of reducing the material strengths directly, the limit length of deviators (ρL) which describes the failure surface of material is reduced. In this way, the strength reduction is indirectly implemented by the isotropic shrinkage of the failure surface in deviator plane. The modified SRM can be generally applied on all strength criteria, so called generalized strength reduction method□GSRM. For GSRM, a numerical algorithm was developed and implemented into the self-developed software. The algorithm was verified through test examples and the obtained results were compared with analytically calculated FoS. The global FoS of a concrete dam is calculated by applying GSRM.

Advances in multi-scale, multi-material, and multi-component Topology Optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

3D TOPOLOGY OPTIMIZATION OF TWO-FLUID HEAT EXCHANGERS

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ABSTRACT

In this study, we introduce an approach to topology optimization (TO) for a two-fluid heat exchanger, specifically designed for additive manufacturing. The design is bifurcated into the header and the core. The header aims to enhance flow uniformity and reduce the pressure drop, while the core is focused on improving heat transfer efficiency. In the core optimization, a concurrent optimization of three materials – hot fluid, cold fluid, and solid – is undertaken using two density fields. An overlap constraint on the dilation fields of these densities ensures the formation of a solid layer between the fluids. The minimal thickness of this layer and the self-supporting angle of the design are regulated by two optimization parameters and a Projected Undercut Perimeter (PUP) based overhang angle constraint [1], respectively. A numerical example showcases the use of a two-density method in designing a heat exchanger core unit cell. Compared to a benchmark straight pipe heat exchanger, our TO design, with a similar volume fraction, demonstrates a significant increase in heat transfer rate. This improvement is credited to the TO design's solid fins which increase the contact area, enhance mixing by splitting and merging flow streams, and reduce pressure drop with aerodynamically efficient structures. In optimizing the header, a hierarchical scheme distributes hot and cold fluids from their single inlet pipes to multiple outlets, optimizing from macro to micro scales. This results in a composite design of varying scales. The same two-density method and PUP constraint are applied, with the modification being a cost function focused on minimizing pressure drop. The final assembly of the heat exchanger integrates the optimized core and header, exemplifying the efficacy of multi-scale, multi-material, multi-component TO in additive manufacturing. This approach not only significantly enhances heat transfer rates but also demonstrates the potential of topology optimization in complex thermal management systems.

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Mesh-free particle methods for multi-physics problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMPROVED LAGRANGIAN COHERENT STRUCTURES WITH MODIFIED FINITE-TIME LYAPUNOV EXPONENTS IN THE PIC FRAMEWORK

Zhihao Qian[*1], Moubin Liu[1], Lihua Wang[2] and Chuanzeng Zhang[3]*

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ABSTRACT

The technique of identifying Lagrangian Coherent Structures (LCSs) has emerged as a powerful tool for studying incompressible flows. Yet, the discrepancies arising from incompressibility assumptions often compromise the accuracy of LCSs constructed using Lagrangian particle methods. In this study, we introduce a modified framework to compute Finite-Time Lyapunov Exponents (FTLEs), addressing the misalignment between the fully incompressible assumption of LCS theory and the inherent incompressibility loss in simulations of particle methods. We begin by examining the correlation between the minimum and maximum FTLEs. By incorporating the deformation gradient and Cauchy-Green strain tensor which account for the time-advancing errors of incompressibility based on continuum theory, we enhance the computational accuracy of FTLEs. Moreover, we introduce the modified FTLE algorithm to the incompressible particle-in-cell (PIC) method for resolving free surface flows and fluid-structure interaction problems. Finally, numerical examples including the Tayler-Green vortices, water sloshing with baffles, an eccentric box sinking in water, and three-dimensional shear-driven cavity problems with high Reynolds numbers are tested to validate the effectiveness of the modified FTLE algorithm and the improved LCSs. These results demonstrate that the proposed modification scheme adeptly counteracts the errors caused by incompressibility loss, enabling accurate computation of FTLEs and detection of LCSs.

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INVESTIGATION OF CAVITATION BUBBLE DYNAMICS NEAR A SOLID WALL WITH PRE-SET BUBBLE BY THREE-PHASE SHARP-INTERFACE METHOD

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ABSTRACT

Cavitation near a solid wall might induce erosion due to the strong pressure and the high-speed jet emanating from the collapse. Previous studies demonstrated that the pressure distribution and the jet pattern during cavitation collapse changed significantly in the presence of a pre-set bubble, offering a potential strategy for reducing surface erosion [1]. In this work, a three-phase sharp-interface method is employed to investigate the dynamic behavior of a single cavitation bubble in the vicinity of a horizontal wall during its expansion and collapse [2]. In contrast to diffusion interface methods, the level set method for handling three-phase topological changes is considered, where surface tension can naturally be taken into account during collapse without considering diffusion effects [3]. A pre-set air bubble is further positioned near the horizontal wall to investigate its effect on the jet during collapse. The influence of the distance between the cavitation bubble and the preset bubble is studied. It is found that the jet generated by cavitation bubble collapse will be away from the wall when the cavitation bubble is distant from the pre-set bubble. However, if the cavitation bubble is close to the pre-set bubble, a high-pressure region is formed in interstitial fluid and the direction of the jet reverses. In addition, the transition mechanism of different collapse mode of the cavitation bubble and the critical distance are analyzed in detail.

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LATTICE BOLTZMANN STUDY OF VAPOR CONDENSATION IN 2D POROUS MEDIA

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ABSTRACT

Vapor condensation in porous media is widely applied in engineering fields, such as heat exchangers, seawater desalination, proton exchange membrane fuel cells, etc. It is a complex process involving coupled multiphase flow, phase change, heat/mass transfer in pore structures. In this work, we study the mechanisms of vapor condensation in 2D porous media at pore-scale by utilizing the hybrid lattice Boltzmann method. First, film condensation on flat surfaces considering various Prandtl and Jacob numbers is simulated and compared with Nusselt's theory, to validate the model. Then, vapor condensation in 2D porous media is studied, considering the influences of temperature difference, porous media structure and surface wettability. The mechanisms of heat transfer, condensation speed, liquid configurations are analyzed and compared under different conditions. This study benefits to improving the understanding of vapor condensation processes in porous media, as well as providing insights to alleviate certain application problems such as water flooding in proton exchange membrane fuel cells, etc.

Recent advances in high-order methods for computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN IMPROVED FLUX VECTOR SPLITTING METHOD FOR CHARACTERISTIC-WISE WENO SCHEMES OF THE EULER EQUATIONS

Jianyu Qin[*1] and Yiqing Shen*[1]

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ABSTRACT

The weighted essentially non-oscillatory (WENO) schemes based on the Steger-Warming (SW) [1] or Lax-Friedrich-type (LF) [2] flux vector splitting methods are extensively applied in simulations of compressible flow fields. Due to the less dissipation, SW method is preferred in flow calculations that require fine scale structures such as direct numerical simulation of turbulence. However, this paper shows that, even if the characteristic-wise WENO scheme is used, SW method may still exhibit oscillations near contact discontinuities. We give a similar analysis as in [3] and show that, in certain situations, the SW method may make the characteristic-wise WENO scheme become close to the component-wise WENO scheme. Then, we propose an improved flux vector splitting method. Its basic idea is that, in the characteristic-wise WENO procedure, an adjusted characteristic speed is used for the flux splitting. Numerical experiments show that the proposed method can keep the non-oscillatory property near discontinuities as LF method and maintain the low dissipation as original SW method in other regions.

Keywords: Flux vector splitting, Characteristic-wise WENO scheme, Contact discontinuity, Low dissipation

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Multiscale Theory and Modeling of Advanced Nanocomposites
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

UNDERSTANDING THE INTERFACIAL CREEP OF FIBER-MATRIX INTERFACE USING MOLECULAR DYNAMICS SIMULATIONS

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ABSTRACT

Creep performance is a crucial parameter for evaluating the long-term effectiveness of composite materials. The interface between fibers and the epoxy matrix significantly influences creep resistance and stress transfer within the composite structure. Over the service life, carbon fiber-reinforced polymer (CFRP) and glass fiber-reinforced polymer (GFRP) exhibit distinct creep resistance properties under sustained loads. This study aims to elucidate the nanoscale mechanism underlying the differences in creep performance between CFRP and GFRP. Interface models of carbon fiber/epoxy and glass fiber/epoxy composites are constructed, the creep evolution of CFRP and GFRP interface models are compared under various loading levels using molecular dynamics simulations. The results reveal that CFRP demonstrates a higher shear threshold under equivalent holding load conditions. Additionally, an energy method and bond autocorrelation function are employed to characterize the differing creep response processes of CFRP and GFRP at the microscopic scale. These findings provide insights into the molecular-level distinctions in interfacial creep behavior between carbon fiber/epoxy and glass fiber/epoxy systems, contributing to an enhanced understanding of creep resistance properties in CFRP and GFRP composites.

Recent advances on interfaces dynamics modeling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DROPLET DYNAMICS: A PHASE-FIELD MODEL OF MOBILE CHARGES, POLARIZATION, AND ITS LEAKY DIELECTRIC APPROXIMATION

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ABSTRACT

We present a Poisson–Nernst–Planck–Navier–Stokes–Cahn–Hillard (PNP–NS–CH) model for an electrically charged droplet suspended in a viscous fluid under an external electric field. Our model incorporates spatial variations in electric permittivity and diffusion constants, as well as interfacial capacitance. Based on a time scale analysis, we derive two approximations of the original model: a dynamic model for the net charge (assuming unchanged conductance) and a leaky-dielectric model (assuming unchanged conductance and net charge). For the leaky-dielectric model, we perform a detailed asymptotic analysis to demonstrate the convergence of the diffusive-interface leaky-dielectric model to the sharp interface model as the interface thickness approaches zero. Numerical computations are conducted to validate the asymptotic analysis and demonstrate the model's effectiveness in handling topology changes, such as electro-coalescence. Our numerical results from these two approximation models reveal that the polarization force, induced by the spatial variation in electric permittivity perpendicular to the external electric field, consistently dominates the Lorentz force arising from the net charge. The equilibrium shape of droplets is determined by the interplay between these two forces along the direction of the electric field. Moreover, in the presence of interfacial capacitance, a local variation in effective permittivity results in the accumulation of counter-ions near the interface, leading to a reduction in droplet deformation. Our numerical solutions also confirm that the leaky-dielectric model is a reasonable approximation of the original PNP–NS–CH model when the electric relaxation time is sufficiently short. Both the Lorentz force and droplet deformation decrease significantly when the diffusion of net charge increases.

DATA-EFFICIENT ONE-STEP MECHANICAL DESIGN OF COMPOSITES USING GENERATIVE AI

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ABSTRACT

The distribution of material phases is crucial to determine the composite's mechanical properties. While the entire structure-mechanics relationship of highly ordered material distributions can be studied with a finite number of cases, this relationship is challenging to reveal for complex irregular distributions, preventing the design of such material structures from meeting specific mechanical requirements. The noticeable developments of artificial intelligence algorithms in material design enable the discovery of hidden structure-mechanics correlations, which is essential for designing composites of complex structures. It is intriguing how these tools can assist composite design. Here, we focus on the rapid generation of bicontinuous composite structures and the stress distribution in loading. We find that generative AI, enabled through fine-tuned Low-Rank Adaptation models, can be trained with a few inputs to generate synthetic composite structures and the corresponding von Mises stress distribution. The results show that this technique is convenient in generating massive composite designs with useful mechanical information that dictates stiffness, fracture, and robustness of the material with one model, and such has to be done by several different experimental or simulation tests. This research offers valuable insights for improving composite design to expand the design space and automatic screening of composite designs for improved mechanical functions.

Computational mechanics of soft matter and machines
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MACHINE LEARNING-DRIVEN OPTIMIZATION DESIGN OF HYDROGEL-BASED METAMATERIALS

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ABSTRACT

The deformation of hydrogel-based metamaterials is a complex nonlinear problem involving soft material contact and large deformation. Numerical simulation of such structures is very time-consuming, and the sensitivity is difficult to derive during optimization design, which makes it difficult for traditional gradient and non-gradient optimization methods to achieve efficient design of such structures. To address this problem, an optimization method based on the combination of back-propagation neural network (BPNN) and multi-population genetic algorithm (MPGA) is proposed to rapidly design hydrogel-based metamaterials with specific mechanical properties in this paper. In this method, several dimensionless design parameters are introduced to describe the structural characteristics of the metamaterial. The initial dataset is constructed based on finite element method simulation results, the mapping relationship between design parameters and metamaterial mechanical properties is constructed by BPNN, and the metamaterial with specific effect is efficiently optimized by combining the MPGA. Based on the proposed method, the design of hydrogel-based metamaterials with specific negative hydration expansion effects as well as hydrogel-based metamaterials with zero/negative Poisson's ratio and adjustable stress-strain curves is achieved. Moreover, this method can significantly reduce the amount of calculation, and can effectively avoid falling into local optimum. The results show that machine learning-driven optimization method is an effective means to design hydrogel-based metamaterials.

Key Words: hydrogel-based metamaterial, machine learning, optimization design, negative hydration expansion, negative Poisson's ratio

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ENTROPY STABLE REDUCED ORDER MODELING OF NONLINEAR CONSERVATION LAWS USING DISCONTINUOUS GALERKIN METHODS

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ABSTRACT

We generalize the construction of entropy stable reduced order models (ROMs) for nonlinear conservation laws from finite volume methods (FVM) to high order discontinuous Galerkin (DG) methods. This generalization preserves entropy stability while simplifying the hyper-reduction step by utilizing the Caratheodory pruning for the hyper-reduction of boundary conditions.

TRANSIENT TOPOLOGY OPTIMIZATION METHOD FOR VISCOELASTIC STRUCTURES BASED ON TIME-FREQUENCY DOMAIN CONVERSION TECHNIQUE

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ABSTRACT

Abstract: In engineering design, precision instruments are often required to realize vibration suppression or amplification within a specified time to ensure the rapidity, accuracy and sensitivity of structural response. Therefore, it is of great significance to carry out transient topology optimization design. Viscoelastic materials are often utilized for vibration control because of their excellent damping properties. However, due to the time-dependent nature of the material properties, when the transient response is solved based on Newmark method, its calculation formula and sensitivity analysis are complicated and difficult to achieve. In this paper, the time/frequency domain conversion technology is put forward to solve the problem of transient topology optimization of large-scale viscoelastic structures. Based on the positive/inverse Laplace transform, the transient problem can be solved efficiently in the frequency domain. The specific research work is as follows:
1) Considering the convolution characteristics of viscoelastic constitutive in time domain, Laplace transform is used to convert transient analysis into frequency domain, and the order reduction model and multigrid preconditioned iterative method are adopted to achieve efficient solution;
2) The fast Fourier transform combined with algorithm is used to construct the numerical Laplace inverse transformation to realize the rapid conversion from the frequency domain solution to the time domain solution. The influence of truncation error and algorithm parameters on the conversion accuracy and computational efficiency is studied, and the solution speed, accuracy and stability are analyzed by comparing with the Newmark method in the time domain.
3) The method of first differentiation and then discretization is adopted to solve the sensitivity of the objective function in the frequency domain based on the adjoint method, and then the sensitivity of the objective function in the time domain is solved by the inverse Laplace transform. Finally, the transient response topology optimization design for viscoelastic structure is realized.
Keywords: Time-frequency domain conversion; Inverse Laplace transform; Vibration control; Viscoelasticity; Topology optimization

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Recent advances in discretization techniques for coupled problems in incompressible fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A DECOUPLED, STABLE, AND LINEAR FEM FOR A PHASE-FIELD MODEL OF TWO-PHASE INCOMPRESSIBLE SURFACE FLOW

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ABSTRACT

We consider a thermodynamically consistent phase-field model of a two-phase flow of incompressible viscous fluids. The model allows for a non-linear dependence of the fluid density on the phase-field order parameter. Driven by applications in biomembrane studies, the model is written for tangential flows of fluids constrained to a surface and consists of (surface) Navier–Stokes–Cahn–Hilliard type equations. We apply an unfitted finite element method to discretize the system and introduce a fully discrete time-stepping scheme with the following properties: (i) the scheme decouples the fluid and phase-field equation solvers at each time step, (ii) the resulting two algebraic systems are linear, and (iii) the numerical solution satisfies the same stability bound as the solution of the original system under some restrictions on the discretization parameters. We will provide numerical examples to demonstrate the stability, accuracy, and overall efficiency of the approach. Our computational study of several two-phase surface flows reveals some interesting dependencies of flow statistics on the geometry.

Computational and analytical advances in nonlocal modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NONLOCAL DIFFUSION IN HETEROGENEOUS MEDIA

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ABSTRACT

The wide applicability of nonlocal models in different areas of science (continuum mechanics, biology, image processing, neural networks) has catapulted them to the center of many analytical investigations. In this talk I will present some recent results on nonlocal systems that exhibit heterogeneous behavior via domain operators or boundary conditions. Of particular interest is the study of the limiting behavior of the nonlocal system as the horizon of interaction shrinks to zero. For the emergent system we identify the classical (differential) counterparts and their physical interpretation.

UNCERTAINTY QUANTIFICATION IN LINEAR DYNAMICAL SYSTEMS BY SPLINE CHAOS EXPANSION

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ABSTRACT

This paper leverages recent progress on orthonormal splines for solving uncertainty quantification (UQ) problems from linear structural dynamics. The resulting method, premised on spline chaos expansion (SCE) [1], construes Fourier-like expansion of a dynamic system response of interest with respect to measure-consistent orthonormalized basis splines in input random variables and standard least-squares regression for estimating the expansion coefficients. The SCE proposed is similar to existing polynomial chaos expansion (PCE), but by swapping polynomials for B-splines, SCE achieves a greater flexibility in selecting expansion orders and dealing with subdomains. For this very reason, SCE can effectively tackle stochastic responses that contain locally high fluctuations and that are non-smooth. However, due to the tensor-product structure, SCE, like its polynomial sibling, also suffers from the curse of dimensionality. Numerical results from frequency response analysis of a two-degree-of-freedom dynamic system indicate that a low-order SCE with fewer basis functions eliminates or substantially mitigates the spurious oscillations generated by high-order PCE in calculating the second-moment statistics and probability distributions of frequency response functions [2].

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Multiphase flow and non-Newtonian fluid - Modelling and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VISCOPLASTIC FLOWS IN GROOVED SUPERHYDROPHOBIC CHANNELS: EFFECTS OF ANISOTROPIC SLIP DYNAMICS

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ABSTRACT

Poiseuille flow dynamics of a viscoplastic fluid in channels equipped with a groovy superhydrophobic (SH) wall is revisited. It is assumed that air (gas) fully fills the SH wall grooves, while forming a flat interface with the overlying viscoplastic liquid. The pressure gradient direction can make any arbitrary angle θ with the groove direction, allowing formation of the longitudinal (θ=0), transverse (θ=90) and oblique (0<θ<90) flows. Anisotropic slip dynamics governs the slippery motion on the formed liquid/air interface, for modeling of which a tensorial slip number is used along with the Navier slip law to correlate the shear stress and the slip velocity tensors on the interface. The Bingham constitutive equation is used to model the viscoplastic rheology. Semi-analytical, explicit-form and numerical models are developed to address the flow problem through quantifying the velocity profile, the effective slip length tensor, and the secondary flow field. The effects of the anisotropic slip dynamics on the flow are evaluated by defining an anisotropy number α, which represents the ratio between the components of the slip number tensor. Considering a creeping flow motion, we define six dimensionless parameters for our flow, i.e. the Bingham (B), slip (b) and anisotropy (α) numbers, the groove periodicity length (l), the slip area fraction (φ), and the groove orientation angle (θ). We find the largest/smallest slip velocity for the longitudinal/transverse flow. In addition, the effective viscosity varies with θ, causing an independent problem at any angle θ; this implies that the oblique flow dynamics cannot be directly obtained using the longitudinal and transverse flow solutions (in contrast to the Newtonian flow). For oblique flows, a secondary flow appears normal to the direction of the applied pressure gradient. We calculate the values of θ_max that correspond to the maximum of the secondary flow rate and the effective slip shear component and quantify their variation versus the Bingham number. The increase in the Bingham number is found to cause a continuous decrease in θ_max. Finally, we quantify the onset of no-shear condition at the liquid/air interface, i.e. when an unyielded plug zone appears on the interface.

Computational mechanics for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MELT POOL TEMPERATURE PREDICTION USING VISIBLE LIGHT CAMERA AND MACHINE LEARNING TECHNIQUES IN METAL ADDITIVE MANUFACTURING

Mostafa Rahmani Dehaghani[*1], Pouyan Sajadi[1], Yifan Tang[1] and Gary Wang[1]*

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ABSTRACT

Metal additive manufacturing (AM) is increasingly significant in fabricating complex geometries unattainable with conventional manufacturing techniques. This technology, however, faces challenges in achieving uniform mechanical properties due to uneven microstructures resulting from substantial heat input during the process. Researchers try to model the thermal behavior and then the process-microstructure-property relationship in order to better control the manufacturing process. The melt pool temperature plays a pivotal role as the temperature dictates the cooling rates and thermal gradients, which directly affect the microstructure and thus the product's mechanical properties like strength and ductility. Therefore, knowing the melt pool temperature is crucial in the modeling of the process-microstructure-property relationship and control of the metal AM process.

To measure the melt pool temperature, pyrometers or thermal cameras are most often used. These methods, however, have limitations. Pyrometers often struggle with accuracy due to emissivity variations and their installation can be challenging. Thermal cameras, on the other hand, can be prohibitively expensive and difficult to integrate into existing AM setups.
To overcome the difficulties of these methods, this study innovatively employs visible light cameras as a cost-effective, versatile alternative to conventional temperature monitoring methods. Approximately 24,000 coaxial visible light images were captured from the Laser wire directed energy deposition machine, equipped with a coaxial visible light camera and a pyrometer to record the melt pool temperature, under varying settings of laser power, travel speed, and deposition rate. These images were then used to train and validate convolutional neural networks (CNN), Gaussian process regression (GPR), and artificial neural networks (ANN) models.

The CNN model processed the images directly, while the GPR and ANN models utilized key features extracted from the images, such as melt pool dimensions and intensity, for regression analysis. The CNN model achieved an R-squared value of 0.718, whereas the ANN and GPR models reached higher R-squared values of 0.863 and 0.835, respectively.

In conclusion, this study not only demonstrates the practicality of using visible light cameras in temperature prediction for metal AM processes but also suggests a more cost-effective approach to quality control in manufacturing. The ability to accurately predict melt pool temperature using this method can significantly impact the metal AM industry by providing a reliable and efficient means to link process parameters with the final microstructure and properties of the manufactured parts, ensuring consistent product quality.

Mathematical modeling and simulation for social, environmental, and disaster prevention issues
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NUMERICAL INVESTIGATION OF THE EVOLUTION OF TENSILE STRENGTH OF OIL WELL CEMENT DURING CURING PROCESS

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ABSTRACT

Well cementing involves injecting cement in the annular space between the steel casing and the geologic formation. Maintaining the mechanical integrity of the cement sheath is of high importance throughout the entire lifespan of wells. It ensures the success of the primary cement job, which involves providing structural support to wells and ensuring zonal isolation to prevent oil leakage.
Mechanical failure of the cement sheath within well cement is influenced by several factors including cement characteristics and development of its strength and elastic constants. The knowledge of the early-age properties (e.g. stiffness and strength) of cement sheath throughout curing time, is essential for failure analysis of the cement sheath during its service life. Although the International Organization for Standardization (ISO) and the American Petroleum Institute (API) proposed recommended methods for assessing compressive strengths of oil well cement, there are currently no equivalent standards for evaluating the tensile strength of oil well cement. Without the ability to assess tensile strength of oil well cement accurately and consistently, it becomes very challenging to estimate induced stresses and determine if a given cement mix offers sufficient tensile strength to resist failure and subsequently well leakage. Previous studies have shown that the tensile strength of the cured? cement is about 30 to 50% of its flexural strength. A correlation factor between the tensile strength of cured cement and its flexural strength has been proposed in the form of a coefficient.

To study the correlation between tensile strength and flexural strength of cement during the curing process, a detailed 3D finite element (FE) model has been developed and is presented in this paper. Considering pre-determined Young's and shear moduli, along with measured compressive and flexural strength values from available experiments in the literature, the tensile strength of cement can be estimated and compared with test data. Once validated, the FE model could be used as virtual testing framework (digital-twin) to related tensile strength of cement to its flexural strength throughout the curing process. Application of the developed FE model in assessing the overall integrity of oil wells will be discussed.

Current trends in phase-field modeling and computations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A UNIFYING FINITE STRAIN MODELING FRAMEWORK FOR ANISOTROPIC MIXED-MODE FRACTURE IN SOFT MATERIALS USING A PHASE-FIELD APPROACH

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ABSTRACT

Materials like composite and elastomers have widespread applications in the automobile, aerospace, and civil engineering. The materials are subjected to mixed-mode loading in real-time applications. These materials have anisotropic and hyperelastic nature. The factors influencing mixed-mode fracture in the materials are studied in the study. This study presents a unifying thermodynamically consistent phase field approach with finite strains for mixed-mode fracture modeling in hyperelastic soft materials. The initiation of the crack and its propagation process are modeled using the adopted phase field method based on a power law criterion. A coupled Neo-Hookean model with orthotropic anisotropy is adopted considering volumetric-deviatoric and a tension-compression decomposition. This helps to model the mixed-mode fracture of anisotropic hyperelastic materials. This model is suitable for capturing the overall response of soft fiber-reinforced elastomeric composites and soft biological tissues. The proposed model is validated by conducting fracture tests on elastomers and elastomeric composites. The results obtained are compared with experimental and numerical investigations from literature.

TIME-DEPENDENT RESPONSE OF UNSATURATED POROELASTIC SOILS UNDER SURFACE LOADING

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ABSTRACT

Poroelastic materials are two-phased materials consisting of a solid skeleton with voids saturated with water. These materials accurately represent the time-dependent response of geomaterials, which settle gradually over time under externally applied loading, known as soil consolidation. Poroelastic model considers the fluid flow, and the pressure change within pore spaces during the consolidation process. Typically, poroelastic soils are saturated with water, and the pore air is treated as a part of the fluid phase. However, for unsaturated soils, the air phase could play an essential role in soil consolidation, and it has to be considered separately from the water phase. This paper analyses the time-dependent response of an unsaturated poroelastic half-space under axisymmetric surface loading. The equilibrium equations of unsaturated soils are expressed in displacements, pore water pressure, and pore air pressure. The seepage equations of pore water and pore air obey the generalised Darcy's law. The general solutions of displacements, stresses, pore water and pore air pressure are derived by applying Hankel and Laplace transforms with respect to the radial and time coordinates, respectively.
Numerical solutions are obtained by employing an accurate numerical quadrature scheme for the Hankel transform inversion and Stehfest's scheme for the numerical inversion of the Laplace transform. The accuracy of the present solution is verified by comparing it with existing results for a saturated half-space. Selected numerical results are presented for an unsaturated poroelastic half-space under a vertical patch load applied on its surface to illustrate the influence of the degree of saturation on time-dependent responses of unsaturated soils. In addition, a set of influence functions corresponding to an annular load and an annular fluid pressure applied on the half-space surface is then derived to demonstrate the applicability of the present solution for the analysis of consolidation settlement of a rigid circular foundation.

Imaging-based methods in computational medicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PERSONALIZING NON-INVASIVE BRAIN STIMULATION TREATMENTS USING IMAGE-BASED ANATOMICAL AND COMPUTATIONAL MODELS

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ABSTRACT

Non-invasive brain stimulation (NIBS) technologies are rapidly gaining traction as novel therapies for treatment-resistant psychiatric disorders. NIBS protocols involve administering electrical pulses to the exterior of the head in order to induce therapeutic changes in neural activity. Despite consistent reports of clinical efficacy over the past two decades, NIBS outcomes vary widely across individuals. This has led to questions about the possibility of increasing remission rates by personalizing the site of stimulation (Klooster et al., 2022). Without practical means to directly measure electric fields within the human brain, research efforts to pinpoint stimulated regions have relied on computational modeling. However, the computational cost of constructing personalized anatomical representations of the head, which consists of the scalp, skull, cerebrospinal fluid, meninges, and brain, have challenged these modeling efforts, forcing them into one of two categories: i) reduced-order geometric models, such as multilayer spherical shells, or ii) image-based finite element models of a small number of subjects. Here, we present an automated pipeline for generating personalized finite element models of the head from magnetic resonance imaging (MRI), which we successfully apply to a cohort of 50 individuals with major depressive disorder participating in a clinical trial of transcranial magnetic stimulation (TMS). Our pipeline combines established cortical surface-based image segmentation tools for the brain with recent tools for atlas-based segmentation of the surrounding tissues in order to derive a three-dimensional geometric representation of individual head anatomy from an MRI scan (Dale et al., 1999; Puonti et al., 2020). In addition to ongoing finite element simulation of induced electric fields, we successfully leverage our models to generate subject-specific, first-order estimates of the TMS treatment site on the cortex. During imaging, study participants wear a specially fit cap with a high-contrast gel capsule attached at the target stimulation site. We project the imaged stimulus location orthogonally across the scalp and onto the cortex using the modeled anatomical surfaces. Making repeated estimates from three imaging timepoints, we demonstrate the ability to efficiently localize the treatment center to an average 5.4 mm radius. Furthermore, using established neuroanatomical methods for registering subject-specific brain anatomy to standardized atlases, we provide descriptive anatomical labels of the effective cortical treatment site to aid clinicians and increase interpretability. Together, our automated image-based pipeline provides a framework for adapting treatment protocols in clinical settings and retrospectively studying the effect of treatment site on NIBS outcome.

MODELLING THE EFFECT OF CURRENT COLLECTORS ON STRUCTURAL BATTERY PERFORMANCE

Karthikayen Raju[*1], Sihan Dong[1], Vincent B C Tan[1] and Tong-Earn Tay[1]*

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ABSTRACT

Structural batteries [1] promise multi-functional performance of simultaneous structural load bearing ability and energy storage. This opens an opportunity to maximize volume utilization and mass savings at the system-level for electric vehicles, UAVs, drones and electric flight applications. Structural batteries being relatively new, research on developing electrodes, electrolyte, device architecture, encapsulation that gives the battery load bearing capability are ongoing. In addition, another important aspect to development of structural batteries are their current collectors onto which the active anode and cathode are coated or integrated directly.

The current collectors considered in this work are carbon fibre and their composites. Carbon fibres being a structural reinforcement in polymer composites and being electrically conductive make it an ideal candidate for structural battery current collectors. The resistivity of the current collectors is not uniform due to the distribution of polymer in the composite. The work focuses on numerical study of the effect of current collector parameters such as geometry, resistivity, and imperfections due to manufacturing on the structural lithium-ion battery behaviour. The imperfections due to manufacturing of the current collectors are measured as local resistivity along the various directions of the current collectors. These local resistivity values are input as spatially varying resistivity of the current collectors to the models.

The work investigates the effect of local resistivity on the cell performance with the Doyle Fuller–Newman (DFN) and the Single Particle Model with electrolyte (SPMe) models [2] and compare the results with experimental observations on structural battery pouch cells. The non-uniform distribution of matrix that causes high resistivity in certain regions leads to some low resistance paths for current to flow and resulting in non-uniform lithium intercalation. These models help in understanding the effect of current collectors on structural battery's performance and hence aid in their design.

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Advanced multiscale and adaptive numerical methods for non-linear solids
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ACCURATE MULTISCALE SOLUTIONS TO QUASI-STATIONARY THERMAL PROBLEMS INVOLVING A HETEROGENEOUS HEAT SOURCE

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ABSTRACT

We address the multiscale resolution of a (quasi-)stationary thermal problem with source term on a heterogeneous material. This situation differs from the mechanical computational homogenization framework in that a precise primal solution (temperature) is sought on the Representative Volume Element (RVE) and that a source term (possible heterogeneous at the microscale) is considered. Various Finite Element square (FE2) approaches are reviewed, differing mainly in their treatment of the source on the microstructure. These approaches are analyzed, in particular through a possible parallel with methods based on double-scale asymptotic expansion.

For this problem, the classical FE2 method [2] respects the Hill-Mandel principle and does not impose a source on the microstructure. This approach is of order 1. In the case of low or no insulated inclusions, these approaches are proving to be sufficiently precise. In counterpart, for insulating inclusions, it is essential to consider the local influence of the source to obtain accurate solutions on the microstructure [1]. Recently introduced, the generalized Hill-Mandel [3, 4] principle makes it possible to consider the source on the microstructure in a FE 2 framework. We show that, thanks to this strategy, methods of order greater than 1 can be constructed.

The accuracy of the numerical results obtained by these different approaches is assessed using a direct simulation of the structure discretizing the heterogeneities. This study allows us to conclude that it is essential to consider the complete heat source on the microstructure [4], and not just its fluctuations [3], to obtain a reliable estimate of temperature variations at this scale. Finally, a quasi-stationary FE2 calculation with temporal loading and nonlinear behavior has been successfully carried out. This simulation confirms the importance of considering the generalized Hill-Mandel principle for avoiding underestimating the temperature in the microstructure inclusions.

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Computational and analytical advances in nonlocal modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPLORING NON-LOCAL ELASTICITY: A COMPARATIVE STUDY OF NATURAL VIBRATION FREQUENCIES IN NANOSTRUCTURES

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ABSTRACT

Classical local elasticity theory (CLET) is widely recognized as effective for modeling large scale structural mechanics problems. Nevertheless, at the nanoscale clear discrepancies arise between CLET predictions and empirical observations, since it does not take into account long range interaction contributions. To bridge this gap, the non-local elasticity theory (NLET) emerges as an alternative, a theory proposed advanced by Eringen and Edelen [1]. In this theory, the stress-strain relationship of a particle within the solid not only depends on itself, but the collective assembly of particles in the material aggregate.

Based on Eringen's theory, Polizzotto [2] introduced a two phase non-local elasticity theory. In this formulation, the volume is composed of CLET and NLET phases. The latter uses an attenuation function to include the long range cohesive forces. This function depends on the internal length of the material (l) which is the main non-local parameter. This approach is convenient as it facilitates the finite element formulation of the problem (NL-FEM). In the present work, the non-local natural vibrations behavior for different structures is studied. For this purpose, the first natural vibration frequency using NLET (ηnl) and CLET (ηl) are calculated using a custom implementation of NL-FEM. The simulations include different geometries (cubes, spheres, plates, and beams), domain sizes (R), materials, non-local parameters (l), and boundary conditions.

The obtained normalized frequency response considering the non-local theory (ηnl) does not depend on the material. Furthermore, it does not depend on l or R independently, but instead on their ratio l/R. Therefore, the behavior of ηnl only depends on domain geometry. Additionally, threshold l/R values are determined. A minimum value l/Rmin, from which the CLET holds for vibration analyses, and a maximum l/Rmax when the size of the domain is no longer feasible compared to the internal length of the material. For the range [l/Rmin, l/Rmax] the response for ηnl presents a linear behavior, and the corresponding regressions are presented.

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MLS-SPH-ALE: AN IMPROVED MESHLESS FORMULATION BASED ON RIEMANN SOLVERS

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ABSTRACT

Nowadays, advances in engineering and CFD have led us to face problems with more complex geometries and higher accuracy needs. Mesh-based and meshless discretizations are usually considered as two completely different strategies to solve partial differential equations, and each comes with its own advantages and disadvantages.
Traditionally, mesh – based methods have been employed to solve this CFD problems, but with today's computational facilities, meshless methods have become very popular for dealing with large deformation or complex geometries problems, like free-surface or wave breaking problems.
In this work, we present a high-accurate, stable and low-dissipative meshless method for CFD applications, the MLS-SPH-ALE method. This method can be seen as a generalized meshless method that under certain circumstances and parameters recovers other well-known methods, such as the Smoothed Particle Hydrodynamics method (SPH). Moreover, there is a relation between the MLS-SPH-ALE method and the finite volume method.
The method was developed to overcome some of the grand challenges [3] of traditional Lagrangian SPH methods, like boundary conditions, accuracy and the treatment of the free surface.

The accuracy and robustness of the proposed method are demonstrated by performing tests cases. In these test cases the new methodology will be compared to the traditional kernel-based method of Vila [4].

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Emerging frontiers and methods in digital manufacturing: Modeling, simulation, and beyond
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VISCOELASTIC FREE SURFACE FLOWS: FROM COMPUTATIONAL MODELS TO EXPERIMENTS AND PHYSICS-INFORMED NEURAL NETWORKS

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ABSTRACT

Fiber formation of polymeric materials is an industrial relevant process that involves shear, extensional, and elastic material response. The polymer solution is compressed and sheared in a die and then exhibit die swell, a predominantly elastic response, as the fibers are extruded. Computational fluid dynamics (CFD) models are needed to describe these flows, to inform process design and perform process optimization. However, CFD of viscoelastic flows have both increased complexity and increased computational costs compared to Newtonian flows, since a polymer stress constitutive equation is necessary to describe the polymer rheology. These stress-constitutive equations introduce a tensor unknown to the CFD calculation. Furthermore, constitutive equations that perform well in shear such as an Oldroyd-B model, become undefined at high extension rates.

In this paper, we investigate die swell and CaBER flows of polymeric solutions where there is also a free surface. The viscoelastic equations are discretized using DEVSS-G method with LBB-stable elements for the velocity and pressure spaces and bilinear interpolation for the stress and velocity gradient space. A multimode Phan-Thien-Tanner (PTT) constitutive equations is used for the viscoelastic response. An arbitrary-Lagrangian-Eulerian (ALE) implementation with pseudo-solid mesh motion is used to solve for the location of the free surface. The velocity, pressure, stress, and velocity gradient equations are discretized and solved with a finite element method. A kernel transformation of the conformation tensor for the stress equations is used to improve stability of the method as the fluid elasticity is increased. Die swell data is available for a number of model fluids, with varying viscosities, elasticities, and shear and extensional thinning. Some preliminary work investigating scientific machine learning into our rheological measurements will also be discussed. Physics-informed neural networks (PINNs) are a recently developed numerical technique that augments traditional approaches to fluid mechanics modeling with high-dimensional and heterogeneous data. PINNs provide a robust framework for both forward and inverse problems, spanning problems where the underlying physics are well-described and data is limited, to problems where physics are partially or largely unknown, but rich datasets are available. We will apply a PINNs framework to utilize data from an idealized CaBER experiment.
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Mathematics and algorithms for predictive digital twins (DT)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RANDOMIZED ALGORITHMS FOR BAYESIAN INVERSION AND DATA ACQUISITION IN PREDICTIVE DIGITAL TWINS

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ABSTRACT

A digital twin couples computational models with a physical counterpart to create a system that is dynamically updated through bidirectional data flows as conditions change. Data Assimilation and Optimal Experimental Design (OED) provide a systematic means of updating the computational model and acquiring information as the physical system evolves. This talk will describe scalable preconditioners and solvers for Bayesian inversion using different randomization techniques. The proposed techniques are amenable to parallelization and drastically reduce the required number of model evaluations. We also develop theoretical guarantees on the condition number. Additionally, the talk will describe connections between OED for Bayesian linear inverse problems and the column subset selection problem (CSSP) in matrix approximation and derive bounds, both lower and upper, for the D-optimality criterion via CSSP for the independent and colored noise cases. We demonstrate the performance and effectiveness of our methodology on a variety of test problems such as Burgers and quasi-geostrophic equations.

Recent advances on interfaces dynamics modeling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CONTACT REPRESENTATIONS IN REDUCED INTERFACE MODELS

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ABSTRACT

Contact interactions play a significant role in the dynamic analysis of non-smooth mechanical systems. Yet, incorporating these contacts into the system dynamic model is challenging due to the numerous ways to account for them. This study introduces and evaluates various approaches to contact modelling techniques, emphasizing how different approaches can lead to differences in the results. To this end, a co-simulation setup serves as the primary framework to address the differences in the contact modelling and the corresponding formulations.

In a co-simulation framework, a system is divided into subsystems that exchange information at pre-determined communication points via the interface. Real-time simulations for virtual environments and prototyping would need non-iterative co-simulation, for which stability is often the main problem. The stability behaviour is controlled by how the system elements are coupled. Model-based coupling offers a potential solution for enhancing simulation accuracy and efficiency. It involves using a reduced model of a mechanical subsystem, with the interfacing subsystem, whether mechanical or from another domain, interacting only with this model. A key element is that the reduced model must accurately represent the mechanical subsystem's behavior.

In this context, the reduced model is developed to represent some specific behaviour of a larger-scale system. In the case of interfacing, we are interested in a specific behaviour that is associated with the interface, i.e., how the other subsystem sees the system we intend to represent with the reduced model. Such a reduced interface model (RIM) is usually defined based on the modes of motion, i.e., degrees of freedom, that are characterizing the interface and the way how these degrees of freedom are expressed and parameterized.

The main challenge in developing the reduced models often emerges when the system is non-smooth, i.e., unilateral contacts/articulations and friction are also important to model. In this work, we address challenges in developing a representative reduced order model for a non-smooth mechanical subsystem and propose solutions to incorporate changes in contact states in the RIM. It will be demonstrated how fundamental assumptions in the contact dynamic incorporation can affect the simulation outcome. We will use examples with interfacing mechanical-mechanical subsystems to illustrate these findings.

Data-driven modeling and design of materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INVERSE DESIGN OF SPINODOID STRUCTURES THROUGH BAYESIAN OPTIMIZATION

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ABSTRACT

In this contribution, we propose a general framework to inversely designing mesostructures using structure-property linkages. Typically, large datasets are necessary. Experiments alone are prohibitively expensive. Therefore, computational augmentation is employed to allow for data-driven approaches even in this data scarce regime.

In an iterative procedure (1) mesostructures are characterized by descriptors, (2) effective properties are derived from numerical simulations, (3) structure-property linkages are set up using a Gaussian process, (4) descriptors of new candidate mesostructures are proposed by Bayesian optimization and (5) mesostructures are reconstructed. Steps 2 through 5 are repeated until a desired convergence criterion is reached, e.g., the uncertainty of the structure-property linkage is decreased or a mesostructured with preferable properties is found.

This framework is applied and presented at the example of spinodoid structures. Augmenting a small initial data set by in silico reconstructed spinodoid structures and their simulated effective properties allows for deriving improved structure-property linkages and, thus, finding potentially optimal structures or predicting properties.

Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LIP-FIELD REGULARIZATION OF SECOND-ORDER ANISOTROPIC DAMAGE MECHANICS MODELS

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ABSTRACT

Softening stress-strain responses lead to strain and damage localization. In a numerical context, this translates into an undesirable dependency of the structural response on the spatial domain discretization. Nonlocal enhancements and regularization techniques are employed to address this issue and recover the mesh independence of the structural response.

The "Lip-field" approach [1, 2] falls into the second category of techniques. In this approach, the unknown displacement and damage fields are determined through the alternate minimization of an incremental potential during each time step. In contrast to phase-field models, the "Lip-field" formulation relies on minimizing a local energy potential and incorporates regularization by imposing a Lipschitz regularity constraint on the damage field. This constraint guarantees the boundedness of the damage gradient across the domain and naturally introduces an internal length parameter.

Although this method is appealing for its robust mathematical foundation, only isotropic damage formulations were considered in [1, 2]. However, when modeling quasi-brittle materials (e.g., concrete), it is crucial to account for damage-induced anisotropy. Addressing this within Continuum Damage Mechanics framework can be achieved, for instance, by representing material degradation through a tensorial damage variable [3].

This contribution introduces the first "Lipfield" formulation tailored for anisotropic damage. To characterize the induced anisotropic material behavior, a convex free-energy potential is defined according to [3]. A crucial aspect of the model lies in defining a dissipation potential. This choice is directly linked to choosing a suitable scalar variable subject to Lipschitz continuity. Here, a "cumulative damage" variable λ is introduced, and the potential is expressed in terms of this variable. Spurious localizations are prevented by enforcing the Lipschitz constraint of a function $g(\lambda)$ chosen appropriately, while the anisotropic nature of damage growth is considered through the evolution law.

To demonstrate the feasibility and advantages of an anisotropic damage formulation over a purely isotropic approach, the proposed model is implemented in a finite element code, and several test cases are illustrated.

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PHASE-FIELD MODELING OF CONTACT BETWEEN DEFORMABLE SOLIDS IN FLUID FLOW

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ABSTRACT

Elastic contact in hydrodynamic environments is a complex multiphysics phenomenon and can be found in applications ranging from engineering to biological systems. The motivation for the current work derives itself from ship-ice interactions in Arctic regions during the collision of ships with large ice sheets, the drifting of ice floes and crack propagation in ice. A fully coupled continuum mechanics formulation is a necessity if we wish to capture the dynamic response of the marine vessel navigating ice-covered Arctic waters. This entails the development of a generalized framework capable of handling topological changes and transitioning implicitly from fluid-structure interaction conditions to solid-solid contact conditions.

Given the physical demands of the problem, we adopt a phase-field based fully Eulerian approach to resolve the multiphase and multibody interactions in the system. We employ a stabilized finite element formulation and a partitioned iterative procedure to solve the unified momentum equation comprising solid and fluid dynamics coupled with the Allen-Cahn phase-field equation [1]. The evolution of solid strain in the Eulerian reference frame is governed by the transport of the left Cauchy Green deformation tensor. We introduce a contact force [2] approach to handle smooth elastic-elastic contact based on the overlap of the diffused interfaces of two colliding bodies. The diffuse interface representation ameliorates the issue of discontinuous contact forces in conventional approaches. The implemented model is validated against the classical Hertz model for smooth dry contact and sensitivity studies are carried out for the model parameters involved. We extend the model to resolve contact between multiple elastic bodies immersed in a surrounding fluid. The developed approach obviates the need for solving multiple phase-field equations or reconstructing the solid boundaries at every time step. Using the proposed framework, we demonstrate the collision dynamics between multiple immersed bodies of varying sizes. We also showcase scenarios where active motion control of a specific body allows us to replicate ship-ice interactions.

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Physics-informed machine learning for numerical modelling in engineering and science
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICS INFORMED MACHINE LEARNING (PIML) FRAMEWORK FOR AIR QUALITY PREDICTION

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ABSTRACT

Air pollution leaves a significant impact to both human health and the global climate, requiring robust predictive models for accurate simulation of pollutant dispersion. The concentration of air pollutants exhibits considerable variability across short spatial distances due to diverse emission sources, meteorological conditions, and chemical processes. Existing models, including mechanism-based methods, statistics-based machine learning methods, and chemical transport models, often facing with limitations in capturing the complex atmospheric dynamics. This research aims to evaluate the Physics Informed Machine Learning (PIML) framework for accurate air quality prediction by integrating physical principles and diverse real-world data. The primary objective of the research is to develop a comprehensive PIML model for simulating air pollutant dispersion and transport. Furthermore, a secondary objective involves incorporation of real-world data sources to enhance the model's applicability. Those can be achieved by leveraging the advection-diffusion equation as the governing equation and employing the Eulerian method for spatial predictions. By integrating physical constraints into the learning process, the proposed model aims to improve accuracy by capturing the intricate dynamics involved in the dispersion of atmospheric pollutants. The expected results anticipate a substantial advancement in predictive accuracy for spatial distributions of air pollutants compared to traditional machine learning models. The significance of this research lies in the integration of advection-diffusion equations with PIML, representing a ground breaking approach that combines data-driven techniques with a strong foundation in physics. This innovation holds promise for refining atmospheric pollutant dispersion predictions, contributing to a better understanding of air quality dynamics, and facilitating more effective mitigation strategies for environmental and public health. Overall, the proposed research represents a pivotal step toward developing comprehensive and accurate models to address the increasingly pressing challenges posed by air pollution.

Data-driven methods for modeling complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN INTEGRATION OF NEURAL, PHYSIOLOGICAL, AND BEHAVIORAL OBSERVABLES THROUGH SHARED LATENT DYNAMICS

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ABSTRACT

A fundamental challenge in neuroscience is the general lack of governing laws relating macroscopic variables. With recent strides in the ability to obtain high-dimensional, multimodal recordings from awake animals, there is growing need for physiologically motivated, low-dimensional descriptions of the effective dynamics. Following recent themes in the experimental literature, we have hypothesized the existence of an intrinsic, arousal-related dynamical process whose organism-wide regulation underpins fluctuations observed across diverse neural, physiological and behavioral measurements (Raut et al. 2021 SciAdv; Raut et al. 2023 biorxiv). Motivated from this perspective, we describe a computational framework aimed at constructing probabilistic mappings between such measurements (e.g., pupillometry and brain images) from a latent, low-rank representation of their shared dynamics.

Specifically, we introduce a data-driven approach to parsimoniously link observables that evolve according to a common but unknown dynamical mechanism. This approach is motivated from Takens' embedding theorem, which permits the (topology-preserving) reconstruction of a full-state attractor manifold from a single observable and its time history. Takens' theorem enables a strong prediction – and thus, a challenging test – of our framework: in theory, a single arousal-related observable (e.g., pupil size) should suffice to reconstruct high-dimensional observables, to the extent that a dynamical mechanism is shared. We test this prediction by performing simultaneous pupillometry and widefield calcium imaging in awake mice. The latter reports the large-scale spatial structure of cortical activity, which we hypothesize to be tightly regulated in accordance with arousal dynamics (Raut et al., 2021). We train neural networks (namely, a variational encoder-decoder architecture) to approximate the hypothesized mapping from delay-embedded pupil time series (i.e., a scalar measurement) to (high-dimensional) widefield measurements.

Following this procedure, we are able to reconstruct a surprising extent of cortex-wide spatiotemporal dynamics in awake mice from simultaneously measured pupil diameter. We achieve similar success using a scalar index of behavioral arousal (whisker movement), and in predicting widefield measurements of brain metabolism or hemodynamics, suggesting the ability of our procedure to elucidate low-dimensional generative factors that underlie physiologically diverse, high-dimensional measurements. Finally, we extend this architecture to multimodal, state-of-the-art behavioral and electrophysiological measurements publicly released through the Allen Institute Brain Observatory—successfully demonstrating our ability to integrate diverse experimental data into a unified generative model via mappings from an intrinsic manifold. Our data-driven approach may find application to other settings in which a coarse-grained

process involving a small set of macroscopic variables may parsimoniously capture the dynamics of high-dimensional, nonlinearly-coupled observables.

PARALLEL–ADAPTIVE MESHING IN A SPACETIME DISCONTINUOUS GALERKIN SOLVER FOR WAVE PROBLEMS

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ABSTRACT

We present recent progress at the University of Illinois in implementing parallel–adaptive spacetime meshing techniques in ParaSDG, a scalable spacetime solver for wave problems based on the causal Spacetime Discontinuous Galerkin (cSDG) method. cSDG solvers feature local conservation properties, linear computational complexity in the number of spacetime elements, unconditional stability without stabilization, and powerful space-time adaptive meshing capabilities. In lieu of synchronous time marching, cSDG solvers construct unstructured spacetime meshes according to a causality constraint that localizes the solution process to small clusters of spacetime elements called patches such that the solution on each patch depends only on adjacent, previously-solved elements and initial/boundary data.

This presentation focuses on formulation and implementation of new capabilities for causal adaptive meshing in up to E^3 x R, previously only available in up to E^2 x R. We present localized, dimension-independent algorithms for tent-pitching, refinement, smoothing and coarsening as well as dimension-specific schemes for flip operations, including four distinct forms of flip operations in E^3 x R. A harmonic triangulation procedure governs adaptive meshing to generate quality meshes in the 3D setting with fewer sliver elements. We present a new meshing scheme that delivers a more compact localization with zero refinement propagation.

Advances in computational biomechanics and mechanobiology
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPLORING THE HELIX-COIL TRANSITION IN DNA: A GEOMETRIC THERMODYNAMIC APPROACH

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ABSTRACT

The helix-coil transition in DNA is a fundamental process that involves the transformation of the DNA molecule from a double-stranded helical state to a single-stranded coiled state. This essential phenomenon plays a pivotal role in various biological processes, such as DNA replication and transcription. A comprehensive understanding of this transition is crucial for obtaining valuable insights into the functionality and behavior of DNA. This study introduces an innovative method for investigating the helix-coil transition by employing the principles of geometric thermodynamics.

Geometric thermodynamics is a branch of thermodynamics that uses geometric and mathematical principles to describe the behavior of thermodynamic systems. In geometric thermodynamics, the thermodynamic properties of a system, such as entropy and free energy, are represented as geometric entities. Ruppeiner geometry [1] is a specific type of thermodynamic geometry that associates thermodynamic fluctuations of a system with the curvature of the thermodynamic manifold. In this study, metric and curvature are determined using the free energy derived from the Zimm-Bragg Model [2] of the helix-coil transition which incorporates nearest-neighbor cooperativity. The coordinates of the thermodynamic manifold are defined as temperature and the number of helical segments. Factors such as temperature, pressure, and external forces can significantly alter the geometric configuration of the DNA molecule, thereby influencing the transition. The variations of curvature with temperature and fractional helicity are examined, providing insights into microstructural changes and interaction dynamics during the transition.

The study reveals that Ruppeiner geometry can provide new insights into the underlying physics of helix-coil transition. It enables us to explore the interplay between the physical structure of DNA and the energetic properties that drive its behavior. This interdisciplinary approach not only enhances our understanding of DNA behavior but also opens new avenues for advanced DNA manipulation techniques. Significantly, it proves instrumental in elucidating the intricate connections between microscopic interactions and macroscopic behavior. This framework equips us with a scalar curvature that proves valuable in enhancing our knowledge of life at the molecular level. This study underscores the importance of interdisciplinary approaches in scientific exploration.

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Advanced model order reduction techniques for computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADAPTIVE NONLINEAR REDUCED-ORDER MODELS FOR THREE-DIMENSIONAL TRANSONIC FLOWS

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ABSTRACT

We present a registration-based nonlinear model-order reduction (MOR) method for parametrized three-dimensional transonic flows. For many parametrized partial differential equations (PDEs), linear MOR methods provide rapidly converging solutions; however, for PDEs with discontinuities whose position depends on the parameter, linear MOR methods are ineffective due to the parametric solution manifolds with slowly decaying Kolmogorov N-widths. To mitigate this issue, we introduce a registration-based nonlinear ROM (NLROM) method that uses nonlinear reduced approximation spaces. Our formulation builds on the following ingredients. The first ingredient is transformed solution manifolds associated with transformed PDEs defined on parameter-dependent warped domains where the discontinuities are aligned. The method finds appropriate transformations in the offline stage by locating discontinuities using statistics of a dilation-based shock sensor and then optimizing transformation parameters to align the discontinuities. The second ingredient is the elements of linear MOR---reduced basis, reduced quadrature constructed using the empirical quadrature procedure, and dual-weighted residual error estimate---but crucially applied to the transformed PDEs and manifold. The third ingredient is an adaptive NLROM training procedure which simultaneously constructs adaptively refined meshes, transformations, reduced basis, and reduced quadrature to meet the user-prescribed output error tolerance in an automated manner. We demonstrate the efficacy of the method using three-dimensional transonic flow problems.

Constitutive modeling of complex materials with machine learning and artificial intelligence
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MAPPING STIFFNESS LANDSCAPE OF HETEROGENEOUS AND ANISOTROPIC FIBROUS TISSUE

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ABSTRACT

Biological tissues are complex materials that play essential roles in the structure and function of living organisms, making their characterization a crucial aspect of many fields of study 1. The accurate characterization of mechanical properties of biological structures is vital for understanding the healthy functioning of tissues and diagnosing diseases 1,2. Alterations in mechanical properties, such as stiffness and elasticity, can provide important insights into disease progression, tissue damage, and other pathological conditions. However, due to the heterogeneity and anisotropy of biological fibrous tissues, this task presents challenges and significant uncertainty when characterized only by single-mode loading experiments. In this study, we propose a new method to accurately map the stiffness landscape of fibrous tissues, specifically focusing on brain white matter tissue. Initially, a finite element model of the fibrous tissue was subjected to six loading modes, and their corresponding stress-strain curves were characterized. By employing multiobjective optimization, an equivalent anisotropic material model (Holzapfel-Gasser-Ogden (HGO)) was inversely extracted to best fit all six loading modes simultaneously. Subsequently, large-scale finite element simulations were conducted, incorporating various fiber volume fractions and orientations, to train a convolutional neural network capable of predicting the equivalent anisotropic material model solely based on the fibrous architecture of any given tissue. We adopted a 3D Resnet to predict the strain-stress curve with simulation data from the finite element models. We aimed to map the stiffness landscape of a small part of the white matter tissue by dividing it into homogenized cubes with equivalent directional properties individually determined according to the tissue microstructure by using the developed deep learning model. The method was applied to local imaging data of brain white matter tissue, demonstrating its effectiveness in precisely mapping the anisotropic behavior of fibrous tissue. In the long-term, the proposed method may find direct applications in traumatic brain injury, brain folding studies, and neurodegenerative diseases, where accurately capturing the material behavior of the tissue is crucial for simulations and experiments.

Emerging topology and shape optimization techniques in computational design of materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THERMOELECTROMECHANICAL TOPOLOGY OPTIMIZATION: NON-CONVEXITY STUDIES FOR MULTIPHYSICS PROBLEMS

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ABSTRACT

Thermoelectric devices, capable of harnessing energy from temperature differentials or serving as efficient cooling solutions, have garnered attention for their potential to revolutionize energy recovery and cooling technologies. In comparison to traditional compressor-based counterparts, these devices offer advantages such as miniaturization, lower associated CO2 emissions, and operation under static conditions, resulting in reduced mechanical complexity. Despite these benefits, the current cost per watt - up to 75$/W [1] - of thermoelectric devices surpasses that of compressor-based technologies, hindering their widespread adoption in the market.

While prior studies have employed the SIMP method and assumed the validity of literature pertaining to mechanical systems [2], our investigation reveals that different physics exhibit distinct behaviors under identical optimization parameters. We delve into the evaluation of non-convex objective functions for thermoelectric devices, offering insights applicable to various physics domains and emphasizing the unique considerations for cooling technologies.

The material removal from the TO can lead to mechanical issues during operation or installation. Our study incorporates stress constraints to ensure the reliability of thermoelectric devices after optimization. The interplay between material removal and stress constraints further influences the convergence of the optimization algorithm, a critical that we further analyze.

Throughout the presentation, we discuss the intricacies of applying density-based topology optimization to thermoelectromechanical systems, highlighting algorithm particulars, convergence studies, and showcasing application examples with tangible results. By presenting our findings, we aim to contribute to the advancement of thermoelectric technology, making it more attractive to the market by concurrently improving efficiency and reducing overall costs.

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Isogeometric methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN OVERVIEW OF ADVANCED ISOGEOMETRIC SIMULATIONS INVOLVING COMPLEX GEOMETRIES

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ABSTRACT

Isogeometric Analysis (IGA) is a successful simulation framework originally proposed by T.J.R. Hughes et al., in 2005, with the aim of bridging Computational Mechanics and Computer Aided Design. In addition to this, thanks to the high-regularity properties of its basis functions, IGA has shown a better accuracy per degree-of-freedom and an enhanced robustness with respect to standard finite elements in many applications - ranging from solids and structures to fluids, as well as to different kinds of coupled problems - opening also the door for the approximation in primal form of higher-order partial differential equations. After a concise introduction of the basic isogeometric concepts, this lecture aims at presenting an overview of some recent advances in IGA with a special focus on problems involving complex geometries, where the characteristics of IGA seem to be of great advantage. In particular, applications that will be discussed include structural and fluid-structure interaction simulations in different contexts ranging from Civil and Mechanical Engineering to Biomechanics, electro-mechanical simulations for biological tissues, and studies on the effect of mechanically-induced stresses on cancer growth.

Recent advances in discretization techniques for coupled problems in incompressible fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LOCAL CONSERVATION LAWS OF CONTINUOUS GALERKIN METHOD FOR THE INCOMPRESSIBLE NAVIER–STOKES EQUATIONS IN EMAC FORM

Leo Rebholz[1] and Maxim Olshanskii*[2]

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ABSTRACT

We consider {\it local} balances of momentum and angular momentum for the incompressible Navier-Stokes equations. First, we formulate new weak forms of the physical balances (conservation laws) of these quantities, and prove they are equivalent to the usual conservation law formulations. We then show that continuous Galerkin discretizations of the Navier-Stokes equations using the EMAC form of the nonlinearity preserve discrete analogues of the weak form conservation laws, both in the Eulerian formulation and the Lagrangian formulation (which are not equivalent after discretizations). Numerical tests illustrate the new theory.

Multiscale Theory and Modeling of Advanced Nanocomposites
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MECHANICAL PROPERTIES OF GLASSY POLYMER NANOCOMPOSITES VIA ATOMISTIC AND CONTINUUM MODELS: THE ROLE OF INTERPHASES

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ABSTRACT

The effect of interphases property on the mechanical behavior of silica–polybutadiene polymer Nanocomposite (PNC) is investigated via combined homogenization and molecular dynamics simulation. In the current work, we propose a multi-scale computational methodology consisting of detailed microscopic simulations and continuum modelling (homogenization) approaches for predicting the spatial distribution of the mechanical properties in polymer nanocomposites (PNC). The homogenization methodology is based on a systematic nano/micro/macro coupling between detailed atomistic molecular dynamics (MD) simulations and the variational approach based on the Hill-Mandel lemma. The model system we studied glassy-PB/silica NC's for different volume fraction of NP. Using MD simulations, the polymer/NP interphase in PNCs is directly examined by probing the distribution of the density and the stress profile at equilibration. The effective Young modulus and poison ratio of the interphases are calculated from the relation between the local stress and strain showing high rigidity in compared to the bulk material . The mechanical properties at the interphases and the polymer matrix are used, together with homogenization approach, to develop a continuum model for the prediction of mechanical properties of the PNC. A good agreement be-tween the calculated effective mechanical properties through MD and continuum models is observed. Although using an appropriate interphase model within micromechanical model is of high importance, the high accuracy should also be considered. To address such challenge and requirements, we present a closed-form analytical model to estimate the mechanical properties of interphase zone, through the molecular dynamic simulation without the aid of any continuum model. Moreover, the mechanical properties of interphases are investigated at different position between the NP and the matrix region in order to ensure the continuously changes from the nanosilica properties to the polymer matrix properties.

Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ROLE OF COMPUTATIONAL MECHANICS AND RECENT ADVANCES

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ABSTRACT

This lecture will focus on the role of computational mechanics in research and applications, followed by an introduction to the Dual Mesh Control Domain Method (DMCDM) that the author has conceived and advanced in recent years. The development of realistic mathematical models of physical phenomena is a part of scientific investigation, which requires the translation of the mathematical models into meaningful discrete models that enable us to systematically evaluate various parameters of the mathematical model and hence the physical process. Mathematical model development and numerical simulations are aids to designers, who seek to maximize the reliability of products and minimize the cost of production, distribution, and repairs. Computational methods can be used to investigate the effects of various parameters of the system on its response to gain a better understanding of the system being analyzed. Thus, the role of computational mechanics is vital to the technological advancement of any society. Currently, the finite element method (FEM) and finite volume method (FVM) are the most commonly used numerical methods for the solution of differential equations, with FEM dominating solid and structural mechanics and FVM witnessing popularity in heat transfer and fluid mechanics. Both methods suffer from certain drawbacks. In 2019, Reddy [1] introduced a numerical approach termed the dual mesh control domain method (DMCDM), which utilizes the desirable features of the FEM and FVM. In the DMCDM the dependent variables are approximated using finite element interpolation functions (as in the FEM), and the governing equation is satisfied in an integral sense over a typical control domain of the dual mesh (as in the FVM). In this lecture, the DMCDM is explained and its application to a variety of linear and nonlinear problems is presented to illustrate the workings of the DMCDM [2].

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Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DISCONTINUOUS FAILURE IN MICROMORPHIC ELASTIC-DEGRADING MODELS

Pamela Reges[*1], Roque Pitangueira[1], Leandro Silva[1] and Lapo Gori[1]*

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ABSTRACT

Structural rupture is triggered, typically, by a localized failure that corresponds to a loss in the material continuity within a specific region of the body. This localized failure is preceded by a well-known phenomenon so-called localization of deformations. This phenomenon holds particular significance in the numerical modeling of the physically non-linear behavior of quasi-brittle materials, which exhibit a strain-softening behavior. Localization is traditionally analyzed from the perspective of acceleration waves, also referred to as waves of weak discontinuities. The existence conditions for the propagation of acceleration waves are linked to the strong ellipticity condition of the equilibrium equations, which can be reduced to an algebraic problem: the spectral problem for an acoustic tensor. This study investigates discontinuous failure within the framework of micromorphic media [1, 2], which is well suited for modeling microstructured materials and also recognized in the relevant literature for its regularization properties due to its non-local formulation. Based on the concepts of propagation of acceleration waves, the acoustic tensor for the micromorphic medium is here derived. The acceleration wave is treated as a propagating surface across which, within small deformations, the second spatial and time derivatives of the displacement vector and the small micro-motion second-order tensor may undergo jump discontinuities. A generalized tangent acoustic tensor is here proposed building upon a recently proposed formulation for elastic degradation in micromorphic media [3], defined in terms of a loading function, generalized secant relations, degradation rules, and a hardening-softening law. The derived acoustic tensor is also specified for the particular case of associated scalar-isotropic damage models. The localization condition for micromorphic media is based on the analysis of the proposed generalized acoustic tensor and the numerical investigation is conducted in the open-source software INSANE, with the development code freely available at the Git repository http://git.insane.dees.ufmg.br/insane/insane.git).

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Computational methods for wind energy
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

WIND FARM STRATIFIED FLOW SIMULATIONS WITH ACTUATOR LINE METHOD AND VARIATIONAL MULTISCALE FRAMEWORK

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ABSTRACT

In this work we present the extension of the actuator line method coupled with the residual-based variational multiscale (ALM-VMS) formulation, originally developed in [1], to model multiple wind turbines under atmospheric flow conditions. Finite element method is used for spatial discretization. The stratified flow formulation in a context of VMS was originally developed in [2]. The ALM-VMS formulation for stratified flows is first validated by comparing velocity deficit and turbulence kinetic energy in the wake region of a NREL 5MW turbine. Multiple cases with varying rotor and wake refinement regions are studied to explore the sensitivity of the results to mesh size. Next, back-to-back turbine simulation is performed under both stratified and non-stratified flow conditions. A precursor simulation is used to generate realistic turbulent inflow conditions. Finally, the simulation of the Lillgrund farm is performed with wind flow from 222° direction at various turbulent intensity levels. The power generated for each row is compared with available data, and an in-depth analysis of the wake dynamics between the turbines is also examined.

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Computation for energy storage
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SUBSTITUTION EFFECT BY SELENIUM AND TELLURIUM ELEMENTS ON ELECTRONIC STRUCTURES, OPTICAL AND THERMOELECTRIC FEATURES OF FES 2 : DFT + U

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ABSTRACT

The effects of selenium and tellurium substitution on structural, electronic, optical, and thermoelectric properties of FeS compound are investigated using the first-principal calculations and Hubbard potential (U). The phonon dispersion of each structure is simulated to examine the feasibility of the synthesis and evaluate the relative stability. FeS2 is an indirect semiconductor with an energy gap of 1.058 eV. The electronic properties can be tuned by substituting sulfur element with chalcogenide. The outcomes suggest that the band gaps are signifi cantly reduced from 1.058 eV to 0.215 eV after substitution. The absorption ability is improved in various wavelength ranges by exceeding 1.10-6 cm1 for FeTe and FeSTe compounds. Other optical properties such as optical band gap, Urbach energy, and dielectric function in both (xx) and (zz) directions are studied. The thermoelectric features of the studied compounds are strengthened and weakened under the temperature effect. The thermoelectric efficiencies are close to the unity ZT ~ 1. The findings prove that substituting is an extremely promising technique for expanding the predicted structure applications and boosting their thermoelectric devices.

Phase-field modeling: Analytics, benchmarks, and discussions
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FINITE ELEMENT BASED MICROMAGNETIC SIMULATIONS OF HETEROGENEOUS STRUCTURES

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ABSTRACT

Cutting edge permanent magnetic materials such as neodymium-iron-boron (NdFeB) magnets play a crucial role in pushing the efficiency of power conversion devices, including wind turbines, sensors and electric motors to their limits, cf. [1]. Their huge potential to strongly influence current technological and social challenges such as the reduction of carbon dioxide emissions, provides a wide field of research, as their general increase in performance, the substitution of critical elements by harmless substances and the reduction of their required production energy. Here, microstructure engineering offers a promising approach, i.e., targeted influencing of sub-grain structures as grain boundaries or defects, to locally improve the magnetic properties. Thereby, finite element based micromagnetic simulations can be a strong technique to predict the magnetization behavior on fine scales. The FEM is characterized by a particularly flexible and not necessarily regular discretization, which is an advantage compared to other numerical methods for the discretization of heterogeneous microstructures, cf. [2]. The evolution of the magnetization vectors is determined by Gilbert's equation, which merely allows rotations, but no changes in length, cf. [3]. This constraint is enforced via a condensed perturbed Lagrange multiplier, cf. [4]. Within this contribution high-resolution micromagnetic simulations of strongly heterogeneous magnetic microstructures are presented. Thereby, the focus remains on analyzing the influence of grain boundary layers and inhomogeneities within the bulk material that often act as weak spots enabling premature reversal.

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Continuum biomechanics of active systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MICROSTRUCTURE-INFORMED, REGION-SPECIFIC VISCOELASTIC MODELING OF HUMAN BRAIN TISSUE

Nina Reiter[1], Lars Bräuer[1], Friedrich Paulsen[1] and Silvia Budday[1]*

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ABSTRACT

Continuum-mechanics based computational models of the human brain can help to better understand mechanics-related processes of neurodevelopment, injury, and disease. A major challenge is, however, that brain tissue consists of many anatomical regions that strongly differ in their microstructural organization and mechanical response.

In a recent study, we have shown that considering the differences of those anatomical regions is essential to ensure the accuracy of whole-brain simulations [1]. However, calibrating material parameters for multiple brain regions remains challenging: firstly, tissue from all required anatomical regions needs to be characterized mechanically through reliable testing methods. Secondly, in phenomenological material models, the calibrated parameters are often highly sensitive to experimental boundary conditions and cannot be transferred to tissues that differ for example in age or health status from the ones used for calibration. This issue can be overcome with microstructure-motivated material models that have microstructural parameters with a physical meaning. Such parameters could be adapted to account for differences between individuals or changes associated with aging or neurological disease. Here, we present viscoelastic data from multimodal (i.e., compression, tension, and shear), large-strain experiments on healthy, postmortem human brain tissue from anatomical structures in the cerebrum, cerebellum, and brain stem and correlate those mechanical data with microstructural data of the same samples from histological examination. The insights gained from those correlations constitute a first step towards microstructure-informed constitutive models [2] for different anatomical regions of the human brain [3] and lay the groundwork for fully microstructure-based material models for human brain tissue.

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Computational fluid dynamics (CFD) and fluid-structure interaction (CFSI): Methods and Applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

X-MESH FOR MULTIPHASE FLOWS

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[2]Ecole Centrale de Nantes

ABSTRACT

The aim of this presentation is to introduce the X-MESH method applied to multiphase flows.

First, we'll look at the possibility of using elements with zero or near-zero measures in a finite element simulation. We will present results that go beyond the angle condition and show that there is a clear link between the use of zero-size elements and mortar methods.

We will then propose a new version of the X-MESH method, which uses a marker-and-cell representation of interfaces in both 2D and 3D. We will show that marker-and-cell coupled with X-MESH, is a very interesting alternative to the use of levelsets for representing complex evolution of interfaces, not only because it allows us to work on a computational mesh with a fixed topology, but also because, in the case of non miscible fluids, it is possible to guarantee the conservation of the mass of the different phases at machine precision.

Computational mechanics in Canada and China: Current states of shared scientific interests and opportunities for the future cooperation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL PROPERTIES AND APPLICATION POTENTIAL OF THE FINITE VOLUME METHOD WITH WALSH BASIS FUNCTIONS

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ABSTRACT

The finite volume method with Walsh basis functions (FVM-WBF method)[1] is a novel high-resolution numerical method recently developed by the author with the ability to capture discontinuity inside grid. An orthonormal basis set composed of Walsh functions that are characterized by square waves is used by this method to approximate the conservative variables in a control volume with Walsh series expansions which are discontinuous forms rather than the traditional continuous forms. Because of the square wave property of Walsh functions, FVM-WBF method breaks through the limitation on shock resolution imposed by the pre-condition that the flow variables vary continuously inside the control volume. A significantly improvement in resolution has been observed in FVM-WBF method when a sufficient amount of Walsh basis functions are used.

The numerical tests show that the new method not only has the high-resolution performance that captures discontinuities inside grid, but also can obtain higher computational efficiency than the traditional finite volume method. This illustrates that the character of square waves of Walsh functions enables FVM-WBF method to produce some new numerical properties that different from the traditional finite volume method. For example:

1) the scale characteristics similar to geometric multigrid can be observed in the FVM-WBF solution system, because the conservative variables are approximated by Walsh series step-by-step;

2) the compact stencils are provided by the Walsh function series in FVM-WBF method to perform high-order reconstruction;

3) the Walsh basis function coefficients has an inheritable nature. Therefore, the adaptive process can be realized by only involving the coefficients transfer, without introducing additional interpolation or reconstruction calculations.

This paper will analyze the numerical properties and application potential of FVM-WBF method, including naturally providing the compact stencils for high-order reconstruction, the dynamic adaptive and the multigrid acceleration convergence. Finally, several numerical examples are used to test the above numerical performance of Walsh function finite volume method.

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Catastrophic failure mechanics and numerical modelling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INFLUENCE OF SEEPAGE SIMULATION METHOD OF WATER STORAGE PROCESS ON VALLEY DEFORMATION AND WORKING BEHAVIOR OF ARCH DAM

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ABSTRACT

During the construction of the high arch dam, the valley has obvious deformation, which affects the working state of the arch dam. How to reasonably simulate the construction and storage process of the arch dam to make the deformation law and magnitude of the valley closer to the actual situation is of great significance for understanding the actual working behavior of the arch dam and ensuring the safety of the arch dam. Take the arch Jinping Ⅰ arch dam as an example, in this paper, the seepage and stress-seepage coupling of dam abutment rock mass are simulated by different methods to study the effect of valley amplitude deformation on dam working state. The results show that when the traditional method is used to calculate the seepage force according to saturated seepage without considering the coupling of stress and seepage, the valley amplitude deformation shows an expanding state, which is opposite to the measured deformation. If the coupling effect of stress and seepage is considered, the valley amplitude deformation is contracted. At this time, if the conversion between unsaturated and saturated seepage in the initial water storage process is not considered, the shrinkage value is too large when the coupling analysis is carried out with saturated seepage. The correct simulation method should consider the stress-seepage coupling and the conversion between unsaturated and saturated seepage during the initial impoundment. The research in this paper shows the importance of selecting the correct simulation method.

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Data-enhanced multi-model uncertainty quantification and experimental design of complex computational systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SAMPLE EFFICIENT ESTIMATION OF RARE-EVENT PROBABILITIES WITH GAUSSIAN PROCESSES AND NORMALIZING FLOWS

Ashwin Renganathan[*1] and Annie Booth*[2]

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[2]*North Carolina State University*

ABSTRACT

Simulating rare events and computing their probabilities find applications in various fields, including extreme weather event prediction and aircraft certification. In this context, we address the challenge of dealing with an expensive black-box computer model of a system in the estimation, which then involves an intractable integral requiring approximation, such as through Monte Carlo (MC) sampling. While naive MC sampling may incur high variance in the estimators, re-weighting with importance sampling (IS) can mitigate this issue, provided a suitable re-weighting, or "biasing," density is identified. A substantial body of work has focused on constructing biasing densities using a surrogate model. However, the overall probability estimation may still entail a considerable cost of O(1000-10000) queries to the model, which could be prohibitive for certain applications. In response to this challenge, we propose a novel method that demonstrate significantly improved sample efficiency. Specifically, by leveraging adaptive Gaussian process models and normalizing flows, we illustrate that accurate estimation of rare-event probabilities, as low as 1e-12, can be achieved with just O(100) queries to the model, while reducing variance. We validate our approach through experiments on several synthetic test functions and a gas turbine thermal stress analysis problem.

Architected materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NOVEL COMPUTATIONAL APPROACH FOR PREDICTING MICRO-BUCKLING SENSITIVITIES IN ARCHITECTED MATERIALS

David Restrepo[1], David Risk[1], Mauricio Aristizabal[1] and Harry Millwater[1]*

[1]*The University of Texas at San Antonio*

ABSTRACT

Architected Materials (AMs) have attracted attention due to their superior properties and functionalities obtained by exploiting elastic micro-buckling. However, the widespread adoption of AMs has been limited by the difficulty in predicting the onset of micro-buckling, which is highly sensitive to defects and imperfections. Current numerical models for analyzing and designing AMs are deterministic and do not account for unintended imperfections, leading to a lack of confidence in their performance. To address this issue, we present a new computational framework based on Hypercomplex Automatic Differentiation (HYPAD) that allows us to quantify local sensitivities in the onset of instabilities and post-buckling behavior of architected materials. In this talk, we will introduce this method to analyze the sensitivities of discrete structures exhibiting snap-through behavior and continuum elements such as geometrically non-linear shells. Our approach provides insights into the most significant factors affecting the onset of buckling and post-buckling behavior of AMs, enabling the development of surrogate models for uncertainty quantification and accounting for unavoidable uncertainties derived from fabrication, assembly, and actuation.

NUMERICAL ANALYSIS OF EVOLVE FILTER RELAX REDUCED ORDER MODELS (ERF-ROMS)

Jorge Reyes[1], Maria Strazzullo[2], Traian Iliescu[1] and Claudio Canuto[3]*

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[2]*Politecnico di Torina*
[3]*Politecnico di Torino*

ABSTRACT

This talk focuses on the development of the numerical analysis behind regularized reduced order models (ROMs) in computational fluid dynamics. Direct numerical simulations have long been understood to be computationally infeasible for day-to-day simulations in computational fluid dynamics. ROMs have been shown to provide an efficient low-dimensional model that enables fast and accurate simulations.

In the case of under-resolved flows, which is generally the case for turbulent flows, standard ROM accuracy tends to suffer. This results in a large variety of ROMs that use different methodologies to improve accuracy while still ensuring swift computations. Regularization, which is based on spatial filtering, increases the ROM stability and accuracy with negligible computational overhead. In this talk, we consider the evolve-filter-relax (ERF) ROM framework as it relates to implicit methods for the Navier Stokes equations. We analyze the numerical diffusion introduced by the scheme, as well as stability and convergence. Several numerical simulations are presented to support the analysis.

Machine learning methods for multiscale and multiphysics material modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATION OF PHYSICS-INFORMED OPERATOR LEARNING FOR ENGINEERING PROBLEMS AND NONLINEAR CONSTITUTIVE MATERIAL BEHAVIOR

Shahed Rezaei[1], Ahmad Moeineddin[2], Ali Harandi[3], Markus Apel[1], Michael Kaliske[2] and Stefanie Reese[4]*

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[2]*TU Dresden*
[3]*RWTH Aachen*
[4]*University of Siegen*

ABSTRACT

Physics-informed operator learning is a new tool for solving boundary value problems in a parametric way. We introduce a novel approach by defining loss functions for neural networks based on the discretized version of the weak form for the given PDEs and BCs. The loss function in this work is an algebraic equation that significantly enhances training efficiency. A distinctive aspect is our independence from classical solvers like finite element methods for data [1]. Additionally, we applied the concept of physics-informed NN to solve the constitutive relations for nonlinear, path-dependent material behavior. The trained network not only satisfies all thermodynamic constraints but also instantly provides information about the current material state under any given loading scenario without requiring initial data [2].

[1] Integration of physics-informed operator learning and finite element method for parametric learning of partial differential equations
[2] Learning solutions of thermodynamics-based nonlinear constitutive material models using physics-informed neural networks

Machine learning and multiscale modeling for complex materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ESTABLISHING PROCESS-MICROSTRUCTURE-PROPERTY LINKAGES VIA DEEP LEARNING IN ADDITIVELY MANUFACTURED CERAMICS

Mohammad Rezasefat[*1] and James Hogan*[1]

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ABSTRACT

Additive manufacturing techniques for ceramics provide several benefits compared to conventional manufacturing processes. These advantages include enhanced design flexibility, minimized material wastage, reduced manufacturing complexity, and the potential for accelerated prototyping and production phases. The goal of this study is to demonstrate how computational mechanics can be effectively used to correlate the processing parameters of additively manufactured ceramics (AMCs) with their microstructural characteristics and functional performance. Here, we develop and train deep learning models to interpret and predict the mechanical behavior of ceramics based on material's synthetic microstructure. This involves analyzing how different processing methods influence the internal structure of materials and how material’s microstructure, in turn, affect their mechanical properties (e.g., stiffness and strength). To achieve these objectives, our methodology consists of four primary components: i) the additive manufacturing of alumina ceramics using Stereolithography method, ii) experimental characterization and testing, employing various specimen geometries such as compression, indirect tension, and semi-circular bending, under both quasi-static and dynamic conditions, and microstructural analysis through EBSD, SEM, and X-ray computed tomography, iii) performing physics-based modeling (i.e., FEM and MD) to further understand of the material's mechanical and failure behavior, and finally iv) integrating manufacturing, microstructure, and mechanical performance using computer vision-based deep learning models, which are crucial for connecting the detailed aspects of the manufacturing process with the resulting material properties. This framework is notably effective for enabling efficient, high-throughput, and multiscale modeling, it is particularly tailored for application in the field of advanced ceramic materials. In summary, predictive modeling tools, validated and informed by current testing and characterization efforts, are aimed at the design of lightweight, high-performance, multifunctional structures made from additively manufactured ceramics. These advanced structures are anticipated to benefit key industrial sectors, including renewable energy, defense, manufacturing, aerospace, mining, and agriculture.

Continuum biomechanics of active systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THERMO-MECHANICAL MODEL FOR PHOTO-ACOUSTIC IMAGING: A ONE-SIDE COUPLED INCOMPRESSIBLE NEO-HOOKEAN UNI-AXIAL MODEL DEVELOPMENT

Ghader Rezazadeh[*1], Mohammad Azhdari[2], Morteza SeyyedPour[3] and Tim Ricken[3]*

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[2]Urmia University
[3]University of Stuttgart

ABSTRACT

Abstract:
Human tissue imaging is essential in medical diagnostics for early illness identification and therapy planning [1]. Technological advancements have significantly improved the accuracy of diagnosis and expanded our understanding of physiological processes. Improving image quality is crucial for detecting fine details in biological structures. Photoacoustic imaging is a state-of-the-art method that provides exceptional clarity and depth in tissue visualization through the use of laser-induced acoustic waves. To accurately measure wave pressure in this imaging technique, a thorough understanding of the thermomechanical behavior of tissues is essential [2,3]. This study presents a new one-sided coupled thermo-mechanical model for human tissues in the context of photoacoustic imaging. The objective of this study is to improve image resolution. To achieve greater precision in tissue characterization, the model utilizes an incompressible Neo-Hookean uniaxial method. This approach lays the groundwork for future advancements in medical imaging technologies. The proposed model accounts for the complex interplay between thermal and mechanical effects by incorporating an incompressible Neo-Hookean model for heat-induced dynamic motion and a two-phase lag model for one-dimensional heat distribution. This contribution presents a precise and comprehensive method for simulating the complex interaction necessary for researchers investigating the thermomechanical behavior of human tissue in photoacoustic imaging.

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Emerging frontiers and methods in digital manufacturing: Modeling, simulation, and beyond
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA DRIVEN UNSUPERVISED CLUSTERING OF METAL ADDITIVE MANUFACTURING CRYSTALLOGRAPHIC TEXTURE DATA

Aashique Rezwan[*1], David Montes de Oca Zapiain[1], Daniel Moser[1], Michael Heiden[1] and Theron Rodgers[1]*

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ABSTRACT

Metal additive manufacturing (AM) parts often have microstructural features (e.g., high-aspect ratio columnar grains, crystallographic orientation gradients, porosity, etc.) that are not well described by traditional microstructure quantification metrics (e.g., grain size and shape distributions). The large amount of microstructural variation that can occur within different features, thicknesses, and build orientations of an AM part can also be challenging to quantify. This work presents a data-driven approach to quantifying microstructures that incorporates grain morphology, crystallographic orientation and phase information. A combination of generalized spherical harmonics (GSH) to map the crystallographic texture, 2-point spatial autocorrelation for both GSH and phase discretization, and a dimensionality reduction technique (i.e., Principal Component/Auto-encoder) is used to discern the complex microstructural data into human-readable results for comparison. Application of this methodology to an experimental dataset of AM 316L stainless steel demonstrated that the method is sensitive to minor microstructural differences within specimens created with nominally identical processing parameters. The method can identify different part orientations, build batches and outliers present in the process. This method can potentially serve as a tool in detecting AM process changes from EBSD data for quality control applications.

Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

A HYBRIDIZABLE DISCONTINUOUS GALERKIN METHOD FOR COUPLED NAVIER-STOKES AND DARCY

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ABSTRACT

In this talk we will present a strongly conservative hybridizable discontinuous Galerkin (HDG) method for the coupled Navier-Stokes and Darcy problem with Beavers-Joseph-Saffman interface condition. These equations describe the motion of a freely flowing fluid coupled to flow of a fluid in porous media and are used to model, for example, surface/subsurface flows.

The HDG method has various appealing properties. First of all, HDG methods were introduced to reduce the large number of globally coupled degrees for freedom of standard higher-order discontinuous Galerkin methods. This is achieved through hybridization [1]. The HDG method is furthermore well suited for coupled problems: coupling between the Navier-Stokes equations and the Darcy equations across an interface is achieved naturally through HDG facet variables. In addition to these properties, the HDG method that we present is designed such that the discrete velocity is globally divergence-conforming and, in the absence of sources and sinks, pointwise divergence-free, i.e., the method is strongly conservative. These properties are appealing in their own right, but have further interesting consequences, namely, the velocity error is independent of the best approximation to the pressure.

In this talk we will show stability and prove existence and uniqueness of a solution to the discretized stationary [2] and time-dependent Navier-Stokes/Darcy [3] problems. Additionally, we present an optimal, a priori error analysis and demonstrate our theoretical results with numerical examples.

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A WORLD OF PURE IMAGINATION? UNDERSTANDING THE DYNAMICS OF VERTICAL STIRRED MILLS WITHIN CHOCOLATE PROCESSING

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ABSTRACT

While it would be nice to imagine a Willy Wonka world where perfectly smooth chocolate is produced by waterfall, the reality is very different. Cocoa liquor is a particle-laden slurry, and these particles need to be reduced in size to create the smooth texture and desired mouthfeel needed for tasty chocolate. A vertical stirred mill is often used to achieve this, as they have greater specific energy transfer and a smaller physical footprint than other grinding techniques [1]. However, there is still little understanding about its exact dynamics on an industrial scale. This is a problem not just within chocolate, but industry as a whole, as grinding is the most commonly used step in manufacturing. Over half of all manufactured products have at least one size reduction stage during processing [2], and up to 4% of global electricity consumption goes into reducing the size of materials [3].

Simulation has opened a new world of possibility to explore the detail of vertical mills and the talk presents a validated simulation using the Discrete Element Method (DEM) technique and experimental data from particle tracking data. The model is trained and optimised using machine learning and while there are limitations in trying to align complex multiphase systems, a good level of agreement with the experimental results can be reached. The model can also reproduce the dynamics of unseen trials to the same level of accuracy as the initial training set, further validating the optimal conditions and means the model can be used with confidence beyond the experimental trials. This truly unlocks a world of pure imagination in better understanding and optimising the process, improving efficiency and tackling the climate crisis.

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Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ANISOTROPIC GRADIENT-ENHANCED EIKONAL DAMAGE FORMULATION WITH EVOLVING NON-LOCAL INTERACTIONS FOR MODELING QUASI-BRITTLE FAILURE

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ABSTRACT

Finite element analysis of damage in quasi-brittle materials implies using regularization approaches to obtain mesh-independent results. Non-local integral or gradient-type methods are usually applied. In most of these approaches, non-local interactions between material points are supposed to be constant and independent of the mechanical fields. Nevertheless, some pathological issues in these models (e.g., damage diffusion and boundary effects) may lead to incorrect descriptions of the damaging/cracking behavior. Non-local approaches with evolving interactions allow for a better description of damage processes and naturally model damage-to-fracture transition (Ribeiro Nogueira et al., 2022).
The present contribution aims to provide theoretical and numerical aspects concerning regularized anisotropic damage modeling in quasi-brittle materials. Particularly, attention is given to the gradient-enhanced eikonal (ENLG) damage model (Desmorat et al., 2015) based on the derivation proposed by Ribeiro Nogueira et al. (2024) using a micromorphic media framework. This approach considers that damage deforms the space where the non-local equivalent strain controlling damage evolution is computed (space curvature is represented through a damage-dependent Riemannian metric). Non-local interactions are thus reduced when damage occurs and vanish in highly damaged zones. Such an approach can be naturally applied to regularizing isotropic and anisotropic damage models.
Here, a second-order tensorial damage model is assumed, and induced anisotropic evolving interactions are naturally considered via the ENLG formation (both in 2D and 3D). This is essential for accurately describing damage/cracking initiation and propagation. After illustrating the main features of the ENLG formulation, its capabilities to represent experimental findings (e.g., size effect) are evaluated.

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Geometric mechanics formulations and structure-preserving discretizations for continuum mechanics and kinetic models
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THERMODYNAMIC CONSISTENCY AND STRUCTURE-PRESERVATION IN A DISCONTINUOUS GALERKIN METHOD FOR THE MOIST COMPRESSIBLE EULER EQUATIONS

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ABSTRACT

We present a thermodynamically consistent and structure-preserving discontinuous Galerkin method for the moist compressible Euler equations. Our spatial discretisation satisfies the first and second laws of thermodynamics independent of the equation of state used, and additionally conserves tracer variance and energy. These properties are achieved by discretising a skew symmetric form of the moist Euler equations, using entropy as a prognostic variable, summation-by-parts properties of discrete operators and a careful choice of numerical fluxes. We experimentally verify our theoretical results with numerical simulations.

Fluid-structure interaction: Methods and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE IMPORTANCE OF EXPERIMENTAL VALIDATION IN FSI PROBLEMS: RECENT AERO-SERVO-ELASTIC TESTS AT LARGE POLIMI'S WIND TUNNEL

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ABSTRACT

Born in the autumn of 2001, but fully operational since 2023, the large wind tunnel of Politecnico di Mlano turns 20 this year and today it is one of the 4 large research infrastructures of the University. Designed, from the point of view of fluid dynamics, entirely within Politecnico, it is close circuit wind tunnel characterized by a particular design that includes two test sections. The boundary layer section (14m x 4m x 38m), located in the return circuit, is particularly suitable for testing objects subjected to the action of the wind such as bridges, skyscrapers, stadiums and large roofing systems; this section is widely used for research in the wind energy sector. The low turbulence section (4m x 4m x 6m), located as usual between the convergent and divergent parts of the tunnel, is mainly used for aeronautical tests, such as airplanes and helicopters, but not only.
Two characteristics make this wind tunnel especially useful for FSI or more generally speaking aeroelastic testing. At first, the large test rooms allow for testing large scale models, in some cases components at full scale. Second, the flow generation system based on 14 fans for a total of 1.5 MW power is fully protected by a steel grid, so that it cannot be damaged by possible brake of aeroelastic models. During years of activity the wind tunnel has been equipped with dedicated equipment for aeroelastic tests that will be presented in the following. In the last 10 years of activity, a large experience has been acquired in different class of aeroelastic testing such as flutter identification and control, gust load alleviation, limit cycles oscillations. Relevant technologically advanced equipments have been developed to respond to complex aeroelastic problems, such as: a six vanes gust generator to produce the excitation profile to test gust load alleviation systems; a floating ground device embedded under a dummy floor to guarantee free plunge and pitch motions to test half models under 1g + gust loads; a photogrammetric system for motion capturing of large models based on 8 high speed cameras. On the side of this experimental capability, DAER POLIMI developed since many years a suite of different numerical tools at different fidelity level to analyze, optimize and control aeroelastic phenomena. The presentation will present the most relevant experiments carried out in the last years as well as the numerical-experimental correlation results obtained.

Advances in material model calibration for computational solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BAYESIAN OPTIMAL EXPERIMENTAL DESIGN FOR CONSTITUTIVE MODEL CALIBRATION USING FULL-FIELD DIC DATA

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ABSTRACT

Calibration and validation of constitutive models is an essential part of accurate computational simulations, which are increasingly being relied upon for engineering decision-making. Thus, there is a corresponding emphasis on the calibration process—both in terms of efficiency and accuracy—and in establishing confidence in predictions of the engineering problem with a quantified level of uncertainty. In practice, the calibration and subsequent validation of material models is often a discrete, multi-stage process that is decoupled from material characterization activities. As a result, the data which is collected does not always align with the data that is needed for calibration. To address this issue, an integrated workflow for delivering an enhanced characterization and calibration procedure—Interlaced Characterization and Calibration (ICC)—has been developed to improve constitutive calibrations with quantified and reduced parameter uncertainty. This framework leverages Bayesian optimal experimental design (BOED) to optimize the information content gathered from characterization experiments, thus minimizing parameter uncertainty.

This work presents results from a constitutive model calibration performed within the ICC framework. In this example, the load path of a metallic cruciform specimen is optimized in order to obtain the most informative data for calibration of an anisotropic yield surface and isotropic hardening material model. The selection of the optimal load path is segmented into the selection of individual load steps from a pre-determined load path tree. The specimen is deformed within a bi-axial load frame, and full-field digital image correlation (DIC) data and load data are collected for calibration. The high dimensionality of the field data is reduced via principal component analysis, and calibration is performed with Bayesian inference, which provides a quantitative measure of uncertainty on the unknown model parameters. Given a set of possible next load steps, BOED is used to determine which load step to take (i.e. on which arm of the cruciform specimen to impose a positive strain) using the expected information gain (EIG) as a measure of how informative each load step option is predicted to be. The experiment is actively driven through the load path with the highest EIG. Prior to beginning the characterization and calibration cycle, surrogate models are constructed to replace the expensive constitutive model and are built for both the load and displacement quantities of interest. The various advantages and disadvantages of the workflow are discussed along with the prospect for future application.

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Geomechanics of the cryosphere
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING SMALL SCALE PROCESSES IN ANTARCTIC SEA ICE

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ABSTRACT

The Antarctic sea ice, subject to annual freezing and melting, holds a crucial role in the global climate cycle. Notably, satellite observations in the Antarctic region have revealed an unprecedented decrease in sea ice extent every year with lowest in 2023. Projections suggest that ongoing ocean warming and future environmental changes in the Southern Ocean will impact the Marginal Ice Zones (MIZ), BioGeoChemical cycles, and their coupled interactions. The 'pancake' floes are characterized by a porous sea ice matrix housing interstitial brine, nutrients, and biological communities within pores. Both ice formation and salinity are dependent upon ambient temperature. To realistically capture these multi-phasic and multi-component coupled processes, we employ the extended Theory of Porous Media (eTPM) presented in (Ricken et al., 2014). This approach enables the development of high-fidelity models adept at simulating diverse seasonal variations in the region. Crucial variables like salinity, ice volume fraction, and temperature, among others are considered, each having its equations of state. The phase transition phenomenon is addressed through a micro-macro linking scheme. Utilizing a Phase-field solidification model (Thoms et al., 2014) coupled with salinity, the micro-scale freezing processes are modeled and scaled up to the macro level using the eTPM model. The evolution equations for the phase field model follow Landau-Ginzburg order parameter gradient dynamics and mass conservation of salt, facilitating the modeling of salt trapped within the pores. In addressing the biological aspect, we establish a BioGeoChemical flux model for sea ice following (Vancoppenolle & Tedesco, 2017), to simulate algal species within the sea ice matrix. Ordinary differential equations capture environmental factors influencing the growth and loss of distinct BGC components. Processes like photosynthesis, dependent on temperature and salinity, are derived through an ODE-PDE coupling with the eTPM model. Academic simulations and results serve as validation for the mathematical model. These sophisticated models are poised to be integrated into large-scale global climate models, enhancing our understanding of the Antarctic sea ice's role in the broader climate system.

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MULTIGRID-IN-TIME METHODS FOR NONLINEAR OPTIMIZATION OF DYNAMICAL SYSTEMS

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ABSTRACT

Fast methods for nonlinear optimization with differential equations are critical to the solution of optimal control, optimal design and inverse problems in fluid, flight, structural and electrodynamics. To compute a step, based on the derivatives of the cost function and the governing differential equations, conventional methods rely on the forward and backward (adjoint) time evolution of the dynamical system. The serial nature of time stepping introduces an inherent computational bottleneck, resulting in long solution times even for relatively simple problems governed by scalar ODEs. In contrast, matrix-free composite-step sequential quadratic programming (SQP) methods [1,2] offer an interesting alternative. Specifically, they solve a sequence of convex quadratic optimization problems that lead to Karush Kuhn Tucker (KKT) saddle-point systems in which the linearized forward and adjoint time evolutions are fully coupled. This time-domain coupling, combined with the convexity of the quadratic subproblems, enables a multigrid-in-time approach.

To develop our multigrid-in-time method, we express the KKT systems in their block-tridiagonal form, where the diagonal blocks maintain the saddle-point structure on each time interval, and the off-diagonal block expose the time coupling. From the tridiagonal form, we construct block-Jacobi and block-Gauss-Seidel fixed-point schemes. The block-Jacobi scheme is used as the pre- and post-smoother for the proposed multigrid method. This smoother is trivially parallelizable in the time domain. A Symmetric block-Gauss-Seidel (SGS) scheme is used as the preconditioner for a coarse-grid solver based on an inner GMRES iteration. The SGS scheme, which is also investigated in [3], serializes in the time domain, however it is applied to only a handful of coarse-grid time steps. We use the multigrid method as the preconditioner for an outer flexible GMRES (FGMRES) iteration.

We demonstrate excellent algorithmic scalability of the proposed multigrid-in-time approach on nonlinear optimization problems with ODE and PDE constraints. More concretely, scalability extends to (i) the inner coarse-grid SGS-preconditioned GMRES method, (ii) the outer multigrid-preconditioned FGMRES method, and (iii) the overall SQP method. Our results also point to a very mild influence of dynamical system coefficients on the number of FGMRES iterations.

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Advanced materials: Computational analysis of properties and performance
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL SIMULATION OF THE SWELLING AND DESWELLING PROCESS OF GEL

Isamu Riku[*1] and Koji Mimura*[1]

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ABSTRACT

It is well known that the entropy elasticity of rubberlike materials and Brownian motion are described by formally analogous equations as both originated from thermal fluctuations. In rubberlike materials, the shear modulus is conventionally considered to be proportional to the absolute temperature and the proportionality factor is the number density of the polymer chains for an affine polymer chains network model. On the other hand, the self-diffusion coefficient of Brownian motion is described as the product of the mobility and the absolute temperature.

However, for the polymer chains network in a solvent, the interaction between the polymer chains and the solvent molecules occurs and the collective diffusion coefficient of the solvent molecules should be different to the self-diffusion coefficient of Brownian motion. Moreover, the shear modulus of the resultant hydrogel should be dependent on the swelling ratio due to the nonaffine movement of the polymer chains.

Therefore, to investigate the analogy of the equations for the shear modulus of the nonaffine polymer chains network model and the collective diffusion coefficient of the solvent molecules, in this study, the swelling and deswelling process of hydrogel is investigated by the numerical simulations.

16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Advances in discretization techniques, element technology, mesh adaptivity, and solution strategies for inelasticity, localization, and failure

July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ENERGETIC MESH SMOOTHING

Julian Rimoli[*1], Alejandro Mota[2] and James Foulk[2]*

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ABSTRACT

Mesh quality improvement is an integral part of finite element modeling, as the quality of the solution as well as the speed of the solution procedure are generally tied to the quality of the worst element in the mesh. Generally, a mesh improvement solution includes the introduction of a mesh quality measure followed by an optimization process, with most mesh quality measures being based on geometric parameters such as minimum angle, length, Jacobian, etc. In this work, we introduce an energetic measure of mesh quality given by the deformation energy of a reference element mapped to the current mesh configuration, assuming a hyperelastic constitution. In this way, the approach is analogous to a set of connected, equilateral, elastomeric elements subject to the topology of the given mesh and finding their equilibrium configuration. This formulation allows us to adopt traditional solid mechanics methods and techniques to optimize the mesh quality, significantly reducing the burden of the mesh improvement process. We will show results on how randomly generated meshes can be automatically improved using our approach.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525.

AUTOMATED CALIBRATION OF CONCRETE MATERIAL MODEL WITH QUASI-STATIC EXPERIMENTS USING INVERSE APPROACH

Daniel Rios-Estremera[*1], Jean Santiago-Padilla[1], Jesse Sherburn[1] and Andreas Frank[1]*

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ABSTRACT

The U.S. Army's ERDC is the leader for the U.S. Department of Defense in the fields of blast and weapons effects on structures and geo-materials, and civil and military engineering. Recognizing the pivotal role of concrete in these critical domains and broader societal contexts, ERDC is dedicated to conducting thorough research aimed at advancements in numerical modeling for concrete materials. This study introduces an automated methodology for inverse parameter estimation and calibration of a complex concrete material model, utilizing quasi-static experimental data. The methodology involves the integration of the constitutive relationships and finite element numerical modeling to estimate optimal parameters. The constitutive relationships determine the failure surface and the non-linear shear modulus from a suite of triaxial loading experiments. Meanwhile, the numerical model consists of a single element under various loading/unloading conditions that induce a series of stress paths, which are compared to analogous experimental data. Parameter optimization is facilitated through the Dakota software [1] from Sandia National Laboratories. This methodology aims to reduce the time and subject matter expertise required for using and calibrating the material model, while maintaining flexibility to allow adaptation to requirement changes resulting from ongoing material model development. Lower barriers of entry will increase the model's availability and viability to a broader audience in the concrete and geo-materials modeling community.

* Permission to publish was granted by Director, Geotechnical and Structures Laboratory.

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Smart structures – Modelling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STUDY OF WIND-INDUCED VIBRATIONS ON A TRELLIS PYLON CONTROLLED THROUGH AN ACTIVE MASS DAMPER SYSTEM

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ABSTRACT

In recent years, especially because of the diffusion of the 5G internet network, it has become increasingly necessary to develop new solutions (such as smart trellis pylons) to install a growing number of antennas for the transmission of the electromagnetic signals, and to implement or improve the monitoring of existing infrastructure.

Steel truss structures for telecommunications typically have very low damping values, even lower than 1%. Therefore, wind-structure interaction phenomena can generate significant oscillations, leading to structural deterioration, potential disturb of the network signal or, in the worst cases, the collapse of the system and a consequent total interruption of the service.

In this context, a detailed knowledge of the wind loads would allow to perform better structural analysis and estimate the beneficial effects of improvement interventions, such as the installation of a damping system or local structural reinforcements. Unfortunately, the modelling of wind actions induced on these structures is a complex and still open issue, and nowadays the national and international regulations introduce oversized safety factors in favour of safety.

In this article we analyse a 50-meter-high steel trellis pylon located on the top of a mountain, at 1300 meters above sea level, in Liguria (Italy). Several accelerometers and one anemometer on the top were installed on the structure. From the experimental measurements of the wind speed and the relative oscillation of the structure it was possible to estimate the wind loads. Then, a reduced modal model of the pylon, identified from the accelerometer measurements, was implemented in Matlab/Simulink considering only the most significant modes. Finally, an Active Mass Damper (AMD) was modelled, starting from the physical parameters of the motor and the control law, and added on the top node of the structure.

From the numerical simulations it is possible to study the structure behaviour with and without the AMD system, comparing the indexes in terms of tip displacement, most stressed structural elements and acceleration at the antennas (or other critical equipment) installation points.

Advanced numerical methods for the modeling and optimization of coupled dynamical systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HYBRID TWIN OF A VERTICAL AXIS ROTATING MACHINE: MODEL ORDER REDUCTION AND MACHINE LEARNING

Sima Rishmawi[*1], Souheil Serroud[1], Sebastian Rodriguez[2], Francisco Chinesta[2] and Frédérick Gosselin[1]*

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ABSTRACT

Rotating machinery plays a crucial role in various industrial systems, including aircraft, vehicles, machine centers, and turbines. It is essential to evaluate the operational conditions of these machines to ensure safety and plan maintenance. Typically, most shafts in these machines are horizontal. In such cases, the bearing reaction forces can be determined by considering the static radial load resulting from the rotor's weight. However, when the shaft is vertical, the clearance between the shaft and the bearing leads to nonlinear bearing reaction forces that are challenging to calculate. Discretized partial differential equations can be used to represent the behavior of rotating machines, the solutions of which depend on various parameters. Creating accurate numerical models for multi-dimensional systems or systems with multiple parameters can be computationally costly, especially if the systems are non-linear. Therefore, the idea of having a pre-calculated library of solutions that can be used to efficiently calculate the system's response to a wide range of problem parameters is attractive. To accomplish this, we propose a two-step approach. Initially, we use a global solver that operates in the non-linear space-frequency domain. This solver generates a low-rank representation of the solution by employing the Harmonic-Modal Hybrid analysis and the Discrete Empirical Interpolation Method (DEIM). The DEIM technique creates a reduced basis for the non-linear function(s) using either calculated or experimental values, thereby enhancing the efficiency of the computations. Subsequently, the optimized solver is employed to perform rapid offline computations, enabling the construction of surrogate models. These models can then provide real-time predictions of the parameterized dynamic response by using the sparse proper generalized decomposition (sPGD) technique. In the second phase, we gather data from an experimental setup comprising a vertical rotating shaft. This shaft is connected to a fixed bearing at its lower end and a compliant bearing at its upper end. The collected data is then used to construct a correction model based on machine learning. This model aims to minimize the discrepancy between the experimental and simulated outcomes, resulting in an enhanced and more precise hybrid twin of the VARM. This twin finds uses in selecting the most favorable operational scenarios, anticipating malfunctions, and planning maintenance. Additionally, it can determine hard to measure parameter values by selecting a solution from this collection that corresponds to real-time measured data. In the future, this approach can be expanded to encompass the entire hydroelectric power generating unit.

Coupled computational mechanics: Solutions for FSI simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TRACKING INTERFACE CONTACT AND PENETRATION IN EMBEDDED BOUNDARY FLUID-STRUCTURE INTERACTION SIMULATIONS

Erick Rivas[*1], Kevin Wang[1], Emily Guzas[2] and Edwin Lopez Ramos[2]*

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ABSTRACT

Abstract:
Embedded and immersed boundary methods are effective tools for simulating fluid-structure interaction problems involving complex geometry and large structural motion. These methods eliminate the need of mesh motion computation and re-meshing. The tradeoff, however, is that the location of the wetted structural surface needs to be tracked within a non-body conforming fluid mesh at every time step. In this work, we tackle a special scenario involving multiple interfaces that may come into contact and penetrate each other. This type of topological change poses a significant challenge to the robustness of existing interface tracking algorithms that are based on projections and intersection detections. To overcome this challenge, we present a numerical method that applies ray-tracing and flood-fill algorithms to detect interface contact and penetration, directly using the fluid mesh for space discretization. Subsequently, existing interface tracking methods are extended to assign correct material/phase information within new disconnected subspaces resulting from interface penetration. For distributed parallel computation, k-d trees and a scoping strategy are employed at the subdomain level to improve efficiency and scalability. The new interface tracking method is capable of separating different fluid and structural domains, identifying edge-interface intersections within the fluid mesh, and computing the shortest distance from any point in the fluid domain to the fluid-structure interface. The performance of this method will be evaluated through academic benchmark tests and real-world engineering problems. In particular, it will be employed to simulate the unsteady hydrodynamics in dynamic underwater docking applications, where unmanned undersea vehicles are required to approach and interface with other undersea vehicles or submerged structures.

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Advances in neural operators for scientific modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEEP NEURAL OPERATORS FOR DATA-DRIVEN MODELING OF MULTIPHYSICS COASTAL HYDRODYNAMICS

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ABSTRACT

High-fidelity numerical models are commonly used to simulate physical phenomena in coastal and near-shore regions that involve nonlinear interactions between wave hydrodynamics, meteorological, and hydrological phenomena. Despite the tremendous progress in computational resources and methodologies, these high-fidelity models are still computationally expensive and require a significant amount of domain expertise. Moreover, in addition to the high computational cost, the challenges of capturing nonlinear spatial features using unstructured meshes across coupled models and the adoption of various empirical approximations render most of the existing high-fidelity, coupled wave-circulation models ineffective for use in ensemble-based forecasting systems and coastal hazard assessment studies.

In this talk, we will present a deep neural operator framework inspired by the deep operator network (DeepONet) philosophy that can generate fast and accurate predictions of various tidal and wind-driven flows arising in coastal environments. We will explore different neural operator model formulations and demonstrate their merits and drawbacks using a benchmark 1D analytical problem. A reduced-order emulator of a real-world example of 2D tide-driven flow in Shinnecock Inlet Bay, New York will also be presented. Such flows are typically simulated by a coupled system of the depth-averaged shallow water equations and the wave action balance equations, and are parameterized by various combinations of meteorological and morphological conditions. Moreover, a typical design and development pipeline for a model problem will be presented to highlight how such a framework might fit as a general approach for reduced order modeling in multi-physics engineering applications.

CONVERGENCE OF NUMERICAL METHODS FOR THE COUPLED CAHN-HILLIARD AND NAVIER-STOKES EQUATIONS

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ABSTRACT

Modeling multicomponent flows in porous media is important for many applications relevant to energy and environment. Advances in pore-scale imaging, increasing availability of computational resources, and developments in numerical algorithms have started rendering direct pore-scale numerical simulations of multiphase flow in pore structures feasible. This talk presents recent advances in the discretization of phase-field models for systems of two-phase flows. Spatial discretization is based on the interior penalty discontinuous Galerkin methods. Time discretization utilizes a decoupled splitting approach. Both theory and application of the proposed methods to model flows in porous structures are discussed.

Advanced computational mechanics based on data-driven techniques for structure, structural dynamics and aeroelasticity
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NEURAL-NETWORKS TO APPROXIMATE THE CONTACT LAW IN INTERFACE DYNAMICS

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ABSTRACT

A detailed representation of the contact forces generated between components is essential when analyzing the dynamical behavior of complex structural assemblies. Even if the contact law is well understood, computing the contact forces during vibration remains a highly expensive task since opening/closing of contact and friction/stiction transitions can occur when vibration amplitudes are high. Capturing these phenomena precisely requires a very fine mesh to localize the contact and determine its nature. Therefore, a strategy to significantly reduce the computational cost of simulation for such problems would be highly desirable in order to use such simulation in design optimization or for health monitoring.

In this contribution, we propose to first apply a modal reduction on a vibrating system with friction contact. The friction forces conjugate to the modal amplitudes are influenced by the complex distribution of the stiction/friction regions and cannot be analytically derived from the contact law directly. Also, computing such modal friction forces is computationally expensive since, as a discontinuous, nonlinear needs to be evaluated at each degree of freedom at the interface. Hence, we propose to train a neural network in order to learn the contact law related directly to the modal amplitudes. We investigate which neural network topology is the most appropriate to represent the history dependent friction forces. We will then assess if the friction forces given by the trained neural network for the modes can properly reproduce the dynamics of the system with contact during a transient dynamics simulation.

The idea will be benchmarked on a simple academic example and the possibility to extend the method to real engineering problems will be discussed.

PERFORMANCE INCREASES OF HYPERCOMPLEX AUTOMATIC DIFFERENTIATION (HYPAD) IN PHYSICS INFORMED SYMBOLIC REGRESSION

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ABSTRACT

Physics regularized genetic programming symbolic regression (GPSR) is a machine learning method for the discovery of symbolic solutions to differential equations. During the symbolic regression process, model outputs are verified by comparison with known analytical solutions for the differential equation(s) under study. As such, derivatives of candidate functions, typically 1st - 4th order, are required during the solution process. The OTI hypercomplex algebra is implemented to provide fast and accurate derivatives. Numerical experiments with second and fourth order differential equations indicate that OTI's provide up to 42X improvement in runtime compared to a PyTorch implementation with no loss of accuracy. Additionally, AD with the OTI hypercomplex algebra consumes less or comparable memory when compared with PyTorch. In addition, the coding implementation is simple and straightforward making the OTI hypercomplex AD method an excellent choice for implementation in PR-GPSR.

CALIBRATION OF STOCHASTIC AGENT BASED MODELS WITH GAUSSIAN PROCESS SURROGATES AND STEIN VARIATIONAL INFERENCE

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ABSTRACT

Agent based models (ABMs) are procedures governing the evolution of many individual units (agents) which interact in a variety of discrete and nonlinear ways. Collectively, these interactions can yield a plethora of complex stochastic dynamics in individual and population level statistics. Additionally, their particle-based nature results in prohibitive computational costs for simulation. As such, they present a formidable challenge for model reduction, calibration, and uncertainty quantification.

In this presentation, we demonstrate techniques for model reduction and calibration of CityCOVID [1], an epidemiological ABM developed to capture the effects of interventions such as alternative schedules and individual protective behaviors on hospitalizations and deaths in the Chicago metropolitan area during the earliest phases of COVID-19. This ABM simulates several million agents moving and interacting in several million locations. To reduce the needed computational expense to calibrate this model, we present a Gaussian process surrogate and quantify its accuracy and shortcomings. We then outline its use in combination with Stein variational inference, a particle based approximate Bayesian calibration (ABC) technique, to provide approximate posterior distributions for key ABM parameters. We provide a comparison of this calibration approach with baseline ABC and MCMC calibrations. The resulting posterior and pushforward distributions are then presented.

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SPARSE BAYESIAN LEARNING FOR THE OPTIMAL SELECTION OF NESTED MODELS WITH BOTH TIME-VARYING AND TIME-INVARIANT PARAMETERS

Brandon Robinson[*1], Philippe Bisaillon[1], Rimple Sandhu[2], Mohammad Khalil[3], Chris Pettit[4], Dominique Poirel[5] and Abhijit Sarkar[1]*

[1]*Carleton University*
[2]*National Renewable Energy Laboratory*
[3]*Sandia National Laboratories*
[4]*United States Naval Academy*
[5]*Royal Military College of Canada*

ABSTRACT

Dynamical systems in engineering applications and epidemiology typically consider complex time-varying processes that are described mathematically by models consisting of time-invariant parameters. To alleviate difficulties in the implementation and computation of these models, simpler, semi-empirical models are often used. Such modelling approaches retain some basis in the physics of the problem, but also rely on data-driven components to accurately recreate the observed system behaviour. The nonlinear sparse Bayesian learning (NSBL) algorithm has been demonstrated as an efficient algorithm for the optimal model discovery in nested models of dynamical systems with time-invariant parameters and for general nonlinear models where the likelihood function can be computed [1].

There are, however, certain applications in damage detection or infectious disease modelling wherein a subset of the system parameters may vary in time. In such cases, robust algorithms that are capable of jointly estimating the system states, time-varying parameters and time-invariant parameters are required. It has been shown that the complementary use of nonlinear filters for the concurrent estimation of system states and time-varying parameters, and for the evaluation of the likelihood function alongside Markov chain Monte Carlo sampling for the estimation of time-invariant system parameters provides a robust and fully Bayesian framework for the concurrent estimation of time-varying and time-invariant parameters [2].

We consider two examples: (i) damage detection from aeroelastic oscillation data where the degradation of the structure may be manifested as a change in the stiffness while the remaining structural and aerodynamic parameters remain constant, and (ii) tracking the time-varying nature of infection rates of infectious diseases, where clinical parameters such as duration of infection remains relatively constant. Through these examples, we investigate for the first time, how the general Bayesian formulation of the two methods described in Ref. [1] and [2], respectively, permits the simultaneous estimation of time-invariant parameters, time-varying parameters, and optimal nested model structure.
References:
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state and parameter estimation framework for stochastic dynamical systems with combined time-varying and time-invariant parameters. Journal of Sound and Vibration, 118106.

UQ-TTA student paper competition in uncertainty quantification
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SPARSE BAYESIAN LEARNING FOR THE OPTIMAL SELECTION OF NESTED MODELS WITH BOTH TIME-VARYING AND TIME-INVARIANT PARAMETERS

Brandon Robinson[*1], Philippe Bisaillon[1], Rimple Sandhu[2], Mohammad Khalil[3], Chris Pettit[4], Dominique Poirel[5] and Abhijit Sarkar[1]*

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Dynamical systems in engineering applications and epidemiology typically consider complex time-varying processes that are described mathematically by models consisting of time-invariant parameters. To alleviate difficulties in the implementation and computation of these models, simpler, semi-empirical models are often used. Such modelling approaches retain some basis in the physics of the problem, but also rely on data-driven components to accurately recreate the observed system behaviour. The nonlinear sparse Bayesian learning (NSBL) algorithm has been demonstrated as an efficient algorithm for the optimal model discovery in nested models of dynamical systems with time-invariant parameters and for general nonlinear models where the likelihood function can be computed [1].

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We consider two examples: (i) damage detection from aeroelastic oscillation data where the degradation of the structure may be manifested as a change in the stiffness while the remaining structural and aerodynamic parameters remain constant, and (ii) tracking the time-varying nature of infection rates of infectious diseases, where clinical parameters such as duration of infection remains relatively constant. Through these examples, we investigate for the first time, how the general Bayesian formulation of the two methods described in Ref. [1] and [2], respectively, permits the simultaneous estimation of time-invariant parameters, time-varying parameters, and optimal nested model structure.
References:
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state and parameter estimation framework for stochastic dynamical systems with combined time-varying and time-invariant parameters. Journal of Sound and Vibration, 118106.

Modeling, optimization and computational analysis of metamaterials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COUPLING MULTIPLE RESONANCES FOR ENHANCING SOUND TRANSMISSION LOSS OF ACOUSTIC METAMATERIALS

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ABSTRACT

Recent developments in acoustic metamaterials have been focused on broadening the attenuating bandwidth features towards lower frequency ranges, well below 1000 Hz, as well as tackling manufacturing issues. In this context, a multi-resonant layered acoustic metamaterial (MLAM) was proposed as a practical realization for addressing both challenges [1]. The MLAM's layered-based design makes it amenable to large-scale manufacturing and the periodic features of each layer enable the application of computational homogenization models to characterize the sound transmission loss (STL) response [2]. Combining these models with optimization techniques allows to determine realistic MLAM designs that trigger multiple resonances in broad frequency ranges. By exploiting coupling mechanisms these resonances translate into multiple STL peaks that produce a broadband continuous frequency range of attenuation, i.e., without transmission peaks in-between. In this work, the proposed computational homogenization model is presented and applied to the design of different MLAM configurations. The goal is to assess the influence of the number of coupled resonating layers in the STL response of the whole MLAM panel, in terms of increasing the attenuation intensity and the effective frequency bandwidth. The results demonstrate the STL enhancements features obtained from exploiting coupling mechanisms, compared to other acoustic metamaterial configurations based on local resonance phenomena. In this context, the proposed MLAM technology exhibits a great potential to provide an efficient, easy-to-manufacture solution to the sound insulation problem at low frequency ranges.

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Enabling technologies for digital twins: Model reduction and scientific machine learning
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

UNCERTAINTY ESTIMATION OF FOURIER NEURAL OPERATORS AS SURROGATES FOR CO2 STORAGE SIMULATION

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ABSTRACT

Carbon Dioxide Capture and Storage (CCS) in underneath reservoirs plays an important role in mitigating global warming. It represents one key technology to reduce the amount of CO2 in the atmosphere. It involves complex multi-phase flows within a subsurface heterogenous medium, and its operational optimization and design rely on very expensive computational simulations. In order to cope with that, Scientific Machine Learning Surrogates [1] have been used, leading to affordable and accurate predictions on proper time. A critical component of reliable predictions is the ability to provide uncertainty quantification. Here, we systematically estimate uncertainties in such predictions due to building surrogates with limited data [2]. We concentrate the study on Fourier Neural Operators tailored for CCS, and some specific geological scenarios are explored, employing different concepts and algorithms for quantifying epistemic uncertainty [2].

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Computational models and methods for predicting cancer progression and treatment response
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREDICTING LEUKEMIA EVOLUTION AND RESPONSE TO TREATMENT WITH STATE-TRANSITION THEORY

Russell Rockne[*1], David Frankhouser[1], Lisa Uechi[1], Sergio Branciamore[1], Denis O'Meally[1], Jihyun Izarriy[1], Yu-Hsuan Fu[1], Bin Zhang[1], Ya-Huei Kuo[1] and Guido Marcucci[1]*

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ABSTRACT

We predict disease evolution and response to therapy using a state-transition model applied to bulk and single cell RNA sequencing data collected from murine models of acute and chronic myeloid leukemia. We demonstrate how the RNA transcriptome can be used as a sensitive, and patient-specific biomarker of disease by following gene expression profiles in the peripheral blood over time. Using a stochastic state-transition model which represents the transcriptome as a particle undergoing Brownian motion in a potential energy landscape, we estimate the model parameters from the transcriptome dynamics, and use the corresponding probability density function to predict disease manifestation and response to tyrosine kinase inhibitor and chemo therapies. We demonstrate that changes in the transcriptome precede detection of leukemia cells, and that very early changes in the transcriptome state are predictive of disease manifestation and response to treatment. Finally, we show how this mathematical approach may be applied to the clinical management of leukemia in the pre and post transplant settings.

The principal contribution of this work is the development and validation of a predictive, patient-specific model of disease progression and response to treatment derived from the dynamics of the peripheral blood transcriptome. This advances the field of precision medicine by moving beyond fixed sets of genes and provides a dynamic, individualized framework for patient-specific predictions.

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DOI: 10.1126/sciadv.abj1664

Certification of simulations and model adaptation in computational science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADAPTIVE ANALISIS FOR SCATTERING PROBLEMS IN THE CARTESIAN GRID DISCONTINUOUS GALERKIN METHOD

Héctor Navarro-García[1], Pedro Diez[2], José Manuel Navarro-Jiménez[1], Antonio Huerta[2], Juan José Ródenas[1] and Enrique Nadal[1]*

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[2]Universitat Politècnica de Catalunya

ABSTRACT

The Cartesian grid Discontinuous Galerkin method, cgDG, [1] is a novel efficient simulation tool for phenomena governed by hyperbolic PDEs in the time domain. The NURBS-enhanced integration allows cgDG to automatically eliminate model approximation errors. However, the analyst must create appropriate meshes to deal with discretization errors. As the solution varies in time, so does the optimal mesh. Hence, creating optimal meshes is a difficult non-automated task.

In this work, we present a fully automated adaptive analysis strategy based on an explicit error indicator. This strategy considers both, refinement and coarsening of the spatial discretization over time and uses a set of rules to decide where to modify the element size and where to change the polynomial approximation.

Our numerical experience shows that the proposed technique can efficiently compute highly accurate results starting with uniform coarse meshes and with insignificant analyst intervention.

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Computational mechanics in high-strain rate and impact engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE FINITE ELEMENT MODELING OF DYNAMIC SHEAR LOCALIZATION AND FRACTURE IN POROUS PRINTED METALS

A. R. Vishnu[1], Mohammad Marvi-Mashhadi[2], Juan Nieto-Fuentes[1], Federico Sket[3] and Jose Rodríguez-Martínez[1]*

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[2]Helmholtz-Zentrum Hereon
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ABSTRACT

We have developed a multiscale finite element methodology to model dynamic shear localization and fracture in porous ductile metals subjected to high strain rates. Porous microstructures from various additive-manufactured materials, characterized using X-ray tomography analysis, have been integrated into computational models to simulate the collapse of thick-walled cylinders, the crushing of Shear-Compression specimens, and the torsion of thin-walled tubes. The simulations have been compared with experiments on additive manufactured AlSi10Mg and Ti6Al4V to identify the effect of porous microstructure on shear localization and fracture. The calculations have provided new insights on the role of size, shape and spatial distribution of voids on ductile failure under shear-dominated loading.

Advanced numerical methods for the modeling and optimization of coupled dynamical systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

WEIGHT REDUCTION IN DYNAMICALLY LOADED SYSTEMS THROUGH THE EFFECT OF DAMPING IN BOLTED JOINTS

Silas Roediger[*1], Carsten Koenke[1] and Heiko Beinersdorf[1]*

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ABSTRACT

In order to reduce vibration amplitudes, MFPA Weimar is investigating joint damping. The effect is based on the relative displacement between two components between which a surface pressure acts. In this case, the surface pressure is applied by a screw connection. The damping behavior is vibration-dependent and amplitude-dependent. The greater the excitation force, the higher the potential for relative movement and the higher the damping factor. In addition, experimental results show the dependence on the vibration mode. This does not apply to vibrations normal to the joining plane; a certain surface pressure must be applied here in order to maximize the damping factor. In decay tests it becomes clear that it is not possible to approximate the curves due to viscous behavior. Superposition with the friction according to Coloumb occurs particularly in the initial range. The aim is to set up a numerical model in order to be able to take the damping effects into account during the development of components. For this purpose, thin-layer-elements (TLE) are introduced into the joint in FE-simulation and provided with a material law that can represent the energy dissipation, non-linear local damping effects are taken into account. The thin-layer-elements are parameterized depending on the material, surface pressure and surface roughness. It is intended to replace damping, often done by a frequency shift of naturals frequencies via added masses, and thus contribute to lightweight construction.

Modeling and simulation of the electro-chemo-thermo-mechanical interactions in energy transition and energy storage systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HOMOGENIZATION BASED MODELLING OF ELECTRO-MECHANICAL INTERACTIONS IN FLUID SATURATED POROUS STRUCTURES

Eduard Rohan[*1], Vladimír Lukeš[1] and Fanny Moravcová[1]*

[1]*University of West Bohemia*

ABSTRACT

We have in mind metamaterials constituted by fluid saturated periodic electro-active microstructures and consider multi-physical interactions between an elastic or viscoelastic solids skeleton and viscous fluid in the channels. Such heterogeneous structures are exposed to electric field and incident acoustic waves. Due to its piezoelectricity [1], or electrostriction, the solid matrix can deform in response to the electric field locally generated by electrodes embedded in the microstructure. To respect dynamic effects of the flow in bulged pores, where the nonlinear advection term of the acceleration is non-negligible, two time scales are considered and an appropriate time scaling of the fast-slow dynamics is introduced in a proportion to the spatial scaling. To account for acoustic streaming, i.e. the mean flow induced by acoustic waves, the perturbation-based splitting method is employed which relies on the flow fields decomposition in the 0th, 1st, and 2nd order terms reflecting the steady, acoustic and time-averaged parts. Correspondingly this enables to decompose the Navier-Stokes equations into three subsystems. Under the small deformation and linear constitutive law assumptions at the heterogeneity level, the asymptotic homogenization method is applied to derive the macroscopic model and the local problems solved in the reference periodic cell.

The homogenized model can be used to explore functionality of the metamaterials which can serve for fluid pumping, or conversely to energy harvesting. In both cases, the electro-mechanic energy conversion is due to the peristaltic deformation. Using the homogenized model, functionality of such metamaterial structures can be explored, however the model must capture the phenomena associated with the fluid-structure interaction in deforming configurations. For this, the nonlinearity can be approximated by considering deformation-dependent homogenized coefficients. To reduce the computational efficiency, the sensitivity analysis of the homogenized coefficients with respect to deformation induced by the macroscopic quantities is employed, cf. [2]. This enables to avoid the two-scale tight coupling of the macro- and micro-problems typical for the ``FE^2" method. Nonlocal electro-mechanical dynamic interactions are concerned in the multi-scale in space-time, as an extensions of [3].

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Advanced computational modelling of wood, wood-based products, bio-composites, and timber structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTATIONAL MODELLING OF MOISTURE TRANSPORT AND SWELLING IN PAPER THROUGH A MULTI-PHASE FLOW APPROACH

C. Rojas Vega[*1], Marc G.D. Geers[1] and Ron Peerlings[1]*

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ABSTRACT

Paper is a natural material composed of fibers and pores. This porous structure is highly sensitive to fluctuations in moisture content. When paper is used for digital printing, fluctuations in the moisture content may produce a hygroexpansion of the material. If the printing process is not properly controlled, unacceptable deformations may result. In this work, we implement a computational finite element-based model to study the moisture transport and swelling in paper. The porous structure is modelled as a multi-phase material by means of the hybrid mixture theory [1]. This methodology incorporates some characteristics of mixture theory and averaging procedures. Balance equations are presented at the microscale level, and by means of an averaging procedure, the corresponding balances at the macroscale are obtained. An application of the hybrid mixture theory can be found in [2], where a triphasic model was derived to study porous cellulose networks. We adapt this model to study paper. The novelty of our work is that the constitutive relations are derived from physical principles and assumptions at the microscale level. Moisture transport in fibers and pores is modelled using unsaturated flow theory, assuming flow to be driven by chemical potential. The pores are modelled as tubular structures with different radii. These are assumed to be parallel to each other. Water fills the smaller pores first and then the larger pores, which is consistent with the microscopic reality of the problem. By assuming that the moisture transport through the pores behaves according to Darcy's law, we derive the permeability of the porous structure. Moreover, a simple constitutive relation is proposed to study the moisture transport through the fibers. By solving analytically a single fiber problem, we found an expression for the mass exchange between fibers and pores. Swelling and mechanical deformations follow a linear elastic law. The performance of the model is verified by using experimental data on plain paper.

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Biomechanics of hard tissues: From experiments and simulations to clinical applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE CRITICAL IMPACT OF ANTHROPOMETRIC PARAMETERS ON FRACTURE GAP MICRO-MECHANICS - A VIRTUAL TRIAL

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ABSTRACT

The evidence base of surgical fracture care is extremely sparse with only few sound RCTs available. We hypothesize that anthropometric factors relevantly influence the local mechanical conditions inside the fracture gap, thereby interfering with the mechanoinduction of fracture healing. Therefore, we developed a finite element model of a tibia fracture, which acted as basis of an in-silico population (n = 300) by systematic variation of anthropometric parameters. Afterwards, simulations of the stance phase were performed and a correlation between anthropometric parameters and the mechanical stimulus in the fracture gap was investigated.

Analysis of the influence of anthropometric parameters on statistical dispersion between different in-silico trial cohorts with respect to the probability to generate two, with respect to anthropometric parameters statistically different trial cohorts, given the same power assumptions.

The mechanical impact inside the fracture gap correlates with anthropometric parameters; confirming the hypothesis that anthropometric factors are a relevant entity. On a cohort level simulation of a fracture trial showed that given an adequate power the principle of randomization successfully levels out the impact of anthropometric factors. From a clinical perspective these group sizes are difficult to achieve, especially when considering that the trials takes advantage of a „laboratory approach “, i.e. the fracture type has not been varied, such that in real world trials the cohort size have to be even larger to level out the different configurations of fractures gaps. Anthropometric parameters have a significant impact on the fracture gap mechanics. The cohort sizes necessary to level out this effect are difficult or unrealistic to achieve in RCTs, which is the reason for sparse evidence in orthotrauma. New approaches to clinical trials taking advantage of modelling and simulation techniques need to be developed and explored.

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Modeling and simulation of advanced manufacturing processes for metals
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADAPTATION OF A CELLULAR AUTOMATA-BASED GRAIN STRUCTURE EVOLUTION MODEL TO ADDITIVE MANUFACTURING CONDITIONS

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ABSTRACT

The decentered octahedron-based cellular automata (CA) method pioneered by Gandin and Rappaz in the 1990s has been heavily utilized in recent years to predict grain structure and texture in metals produced via additive manufacturing (AM). Under unidirectional and bidirectional scan conditions the method has well-reproduced experimental trends, observed grain structures, and crystallographic textures. However, the predicted textures can be inconsistent with those from parts produced with the common AM scan strategy of rotating the raster scan direction between layers. In turn, this model error may lead to inaccurate prediction of important texture-dependent material properties such as yield stress anisotropy or creep performance. To address these shortcomings, we analyze the key assumptions made in the original decentered octahedron algorithm, which was applied to the solidification of castings. We show that these assumptions lead to error in the competition between solidifying grains at AM melt pool boundaries, as the cooling rates and thermal gradient magnitudes are much larger than those encountered in castings and the interface geometry much more complex. Corrections to the grain envelope advance algorithm are made to account for the large discontinuity in undercooling seen across cell boundaries under large thermal gradient conditions, allowing better resolution of the competition between grains. Additionally, modification of the octahedral grain envelope shape is shown to yield a variety of textures based on input variables governing the transient grain evolution and the grain anisotropy. The modified CA method is shown to enable more accurate texture evolution under complex thermal conditions with large temperature gradients at coarser cell sizes than previously possible. These developments enable more effective and computationally efficient use of CA models in AM process-microstructure workflows. This research has been authored by UT-Battelle, LLC under Contract No. DE-AC05-00OR22725 with the U.S. Department of Energy. Research was co-sponsored by the U.S. Department of Energy Office of Energy Efficiency and Renewable Energy, Advanced Manufacturing Office.

Data-driven approaches for solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A DATA DRIVEN MODEL FOR PREDICTING THE YIELD AND PLASTIC HARDENING BEHAVIOR OF METALS USING BRINELL INDENTATION TESTS

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ABSTRACT

When investigating the mechanical behavior of metals, particularly under large deformations, obtaining the yield and hardening behavior of the material is a crucial step. Usually, this behavior can be found using standard uniaxial tension or compression tests. However, when there is a need for a non-destructive investigation or when no standard specimen can be procured, other, indirect methods are sought after, such as the instrumented indentation test [1-2].

Although prediction of the plastic behavior of metals from instrumented indentation is not new, most modern methods require a continuous load-depth curve of the indentation test. When trying to predict the plastic behavior using a limited number of discrete indentation cases, no significant advancement is reported since the classical work of D. Tabor [3].

In this study, a two-stage data driven model has been developed for predicting the yield and plastic hardening behavior, based on 140 finite element based Brinell indentation tests. From these tests, several indentation force and trace diameter pairs were extracted for each material, and a database of a material's yield and hardening parameters, with its indentation information was constructed. Using this database, an empirical model was developed, which utilized minimization techniques to predict the material's plastic parameters based on their indentation results. The results of this empirical model were then fed to an Extreme Gradient Boosting algorithm to further refine the prediction capabilities. The trained two-stage model was then tested on 30 new numerical and experimental test cases, showing overall better accuracy than the classical Tabor method in predicting both the yield stress of a material, and its hardening curve.

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THE ENERGY-STEPPING MONTE CARLO METHOD: A MARKOV CHAIN MONTE CARLO ALGORITHM BASED ON A SYMPLECTIC, ENERGY-CONSERVING TIME INTEGRATOR

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ABSTRACT

Often, data-driven models require sampling complex, high-dimensional probability distributions. For that, Markov chain Monte Carlo (MCMC) methods are the standard tools. Naïve implementations of these algorithms have a huge cost and thus many optimized methods have been proposed. One of the most popular ones, the Hamiltonian Monte Carlo (HMC) method, transforms the sampling process into a surrogate dynamical problem that needs to be integrated in time. The discrete solution of these trajectories is then interpreted as proposal samples that are later accepted or discarded depending on detailed rules that achieve the desired distribution. The properties of the time integration employed have a crucial impact in the MCMC method, and thus structure-preserving (symplectic) integrators are usually selected.

In this talk, we will present the energy-stepping Monte Carlo (ESMC) method. It is an HMC method where the time-integration phase of the algorithm is performed using the energy-stepping scheme [1], a quasi-explicit structure-preserving method that is symplectic and energy-preserving. As a result of this choice, the new MCMC possesses remarkable properties: in particular, no proposed sample is ever discarded irrespective of the dimensional and complexity of the sampled distribution, hence being more efficient than other HMC.

The talk will describe the theory behind the method, numerical examples showcasing its favorable properties as compared with other MCMC methods, and how the latter can impact data-driven simulations.

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Multiphysics and data-driven modeling for cardiovascular biomedicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A LAGRANGIAN COMPUTATIONAL METHODOLOGY FOR ASSESSING MIXING IN HEMODYNAMIC FLOWS WITH APPLICATION IN CAROTID ATHEROSCLEROSIS

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ABSTRACT

Key Words: Lagrangian method, Particle-based method, Hemodynamics, CFD

Plaque buildup within arteries, referred to as atherosclerosis, poses a critical threat for cerebral embolic events contributing to stroke, which remains the global leading cause of death. Hemodynamics plays a crucial role in etiology of diseases such as atherosclerosis with factors such wall shear stress commonly studied when analyzing the manifestation in local flow changes. However, the ability to gauge disease progression using quantitative hemodynamic factors remains limited. Quantification of mixing within the local region of the disease is widely regarded as an important factor underlying atherosclerotic disease and its susceptibility to progression. The carotid arteries are a common source of embolic events and are prone to the build-up of atherosclerotic plaques in varying degrees. Atherosclerosis results in the reduction of the arterial cross-sectional diameter due to the plaques build up, referred to as stenosis. Identifying quantitative descriptors of mixing in the stenotic arterial environment in a patient-specific vasculature can provide beneficial insights for atherosclerotic disease.

Here, we present a Lagrangian particle-based methodology to quantify mixing across varying degrees bilateral stenosis. Our methodology consists of two computations based on numerically integrated tracer particle trajectories: (a) an entropic measure of fluid mixing within the region of stenosis; (b) Lagrangian Coherent Structures (LCS) identified within Finite Time Lyapunov Exponent (FTLE) fields of the stenosis region. For both, careful resolution of vascular geometry is ensured by using a signed-distance field-based algorithm for particle dynamics. Our entropy descriptor is based on tracking the release of tracers from the surface and the cross-section of the start of the stenosis within the right and left carotid region across varying degrees of disease. The result quantifies the extent of mixing over the cardiac cycle within the stenosed region of the carotid artery. Conversely, LCS allows us to identify regions of deposition within the stenosis that are susceptible to disease progression. We will illustrate the underlying computational framework using a patient-specific case-study with varying bilateral carotid stenosis. Ultimately, our goal is to devise an in silico framework for evaluating atherosclerotic disease progression using Lagrangian-based hemodynamic factors.

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Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MATERIAL CHARACTERISATION PARAMETERS EFFECTS ON TURBINE DISK RUPTURE SPEED PREDICTIONS

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ABSTRACT

Given that turbine disks are massive and turn at high speeds, they contain a significant amount of kinetic energy. Consequently being able to predict when they rupture is important for minimizing fuel burn, and thus reducing emissions while still providing the maximum possible life of part. Thus being able to accurately predict the rupture speed and understanding the uncertainty of these predictions is an active source of study. Furthermore, since running one large turbine disk provides only one data point on the rupture speed with no indication of the margin of error in other highly stressed areas of the disk, experiments have been performed on smaller disks that are designed to fail at each at risk area, providing multiple comparisons to the fracture prediction calculations.

The damage model used in this study takes into account three different modes of rupture. One mode is based on the triaxiality of the stresses, another is a parabolic function of the Lode angle and the final discriminant is the level of necking the material undergoes. The material model is an isotropic continuum material law with an isotropic hardening and a nonlinear kinematic hardening. The material parameters explored are the plastic yield point in the isotropic hardening model and the hardening and saturation variables for the kinematic hardening. Since previous work (Staber, 2021) has indicated that the shape of the plasticity threshold has a significant effect on the prediction of failure a Hosford threshold was used to change between a von Mises threshold and a Hosford value of 6 and 8.

The effects of the material identification is explored using a Maximum projection Latin Hypercube design of experiments. Since the damage model includes the effects necking, lode angle and triaxiality several different geometries, both 2D and 3D were modeled to have a larger sample of stress triaxialities and load angles. The goal of this study is to characterise how the uncertainty in the material definition propagates to the prediction of the rupture speed.

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Volumes 222-223, 2021, 111010, ISSN 0020-7683, https://doi.org/10.1016/j.ijsolstr.2021.02.021.

Data-driven modeling and design of materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A COMPARISON OF APPROACHES FOR THE INVERSE DESIGN OF SPINODOID METAMATERIALS WITH TAILORED STIFFNESS

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ABSTRACT

Mechanical metamaterials or architected materials are becoming increasingly popular due to rapid developments in additive manufacturing. These metamaterials are characterized by mechanical properties that differ greatly from those of the base material and may even exceed them. This is realized with a rationally designed spatial structure of the base material, which allows tuning the effective properties of the resulting solid. In order to efficiently design structures with desired features, it is necessary to invert the relationship between a structure and its properties. While the forward mapping from a given structure to its mechanical properties is well-defined, the inverse mapping from properties to a corresponding structure is ambiguous. This ambiguity makes the inverse problem difficult to solve.

This contribution addresses the solving of such inverse problems in the context of mechanical metamaterials, especially for the relationship between structure parameters and associated stiffness for spinodoid structures. The basis for the presented approaches is a sufficiently large data set of parameter-stiffness pairs obtained from homogenization calculations. Two different methods are examined, that make use of the Lp-adaptation algorithm [1] and invertible neural networks [2]. Lp-adaptation is a stochastic method, that allows to generate robust designs, i.e., designs that meet desired requirements while being as insensitive as possible to small changes in the space of structure parameters. For this purpose, the method only evaluates the forward process, which can be replaced by a standard feed-forward neural network, for example. Invertible neural networks, on the other hand, offer the advantage, that due to their internal architecture, the inverse mapping is automatically available as soon as the network has learned the forward mapping. By introducing additional latent variables in the output of the forward process, the originally ambiguous problem becomes unambiguous and thus invertible. This allows to determine all parameter combinations that result in a desired stiffness with only a single feed-forward network. The quality of the obtained results as well as conceptual advantages and disadvantages of these methods are demonstrated and compared with the literature results from [3].

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Probabilistic learning and constrained generative models for uncertainty quantification
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SPARSE PROBABILISTIC TRAINING OF PHYSICS INFORMED NEURAL NETWORKS IN MECHANICS APPLICATIONS

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ABSTRACT

The discretization of parametric partial or ordinary differential equations describing complex physical phenomena leads to high-dimensional problems, the solution of which requires a massive computational effort. To address this challenge, the development of low-cost surrogates in a data driven manner is the main focus of this talk. To incorporate prior knowledge as well as measurement uncertainties in the traditional neural networks, an efficient sparse Bayesian training algorithm is introduced. By fine tuning specially designed priors the proposed scheme automatically determines relevant neural connections and adapts accordingly in contrast to the classical gradient-like solution [1]. Due to its flexibility, the new scheme is less prone to overfitting, and hence can be used to approximate both forward and inverse maps by use of a smaller data set. The optimal choice of the measurement data then can be easily achieved by maximizing the information gain. In this talk the new type of learning will be showcased on a high-dimensional stochastic partial differential equation describing the nonlinear mechanics problem. The neural network architecture is taken to be of hybrid type being able to describe both time and spatial dependency [2].

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Computational mechanobiology of musculoskeletal tissues
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING BONE MINERALIZATION AS A REACTION-DIFFUSION SYSTEM

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ABSTRACT

Newly formed bone consists of a fibrous, unmineralized collagen matrix. During bone mineralization calcium-phosphate mineral crystals are deposited in the matrix resulting in substantial changes of its mechanical properties. The basic structural units of newly formed bone in compact bone are osteons. These cylindrical structures are approximatively 300 μm in diameter and up to some millimeters in length, with a central Harversian canal accommodating blood vessels and nerves. Osteonal bone is permeated by a network of cavities (lacunae) and channels (canaliculi) housing a cell network (osteocytes) that – among other functions – allows the transport of mineralization precursors into the depth of the osteoid (Raguin et al. 2023) that forms during remodeling of the tissue.
The new osteon starts with the formation of a tunnel by resorption followed by the deposition of osteoid. This is followed by mineralization, which is described as a macroscopic mineralization front moving towards the Haversian canal. Three-dimensional high-resolution imaging using Focused Ion Beam-Scanning Electron Microscopy (FIB-SEM) revealed that the surrounding of canaliculi remains free of mineral over an extended period during mineralization (Ayoubi et al. 2021). This led to the hypothesis that a second microscopic mineralization front – nested in the macroscopic one – moves towards the canaliculus.
We analyzed in a first step the FIB-SEM images to quantify the mineralization pattern around single canaliculi. Different spatial positions along the canaliculi correspond to different time points in the mineralization process. In a second step we developed and explored a reaction-diffusion model generating mineralization patterns due to an interplay between a mineralization precursor and a mineralization inhibitor. Both diffuse simultaneously from the canaliculus, with the precursor turning into immobile mineral when its concentration exceeds the inhibitor's.
The mineralization pattern produced by the model agreed qualitatively with the patterns observed in FIB-SEM under the conditions of a constant flux of precursor and inhibitor from the canaliculus into the matrix. Both larger flux values for the precursor and a lower diffusion constant of the inhibitor ensured a start of the mineralization far away from the canaliculus. Noticeably, the model did not exhibit realistic results when precursor and inhibitor were kept at a constant concentration (as opposed to a constant flux) at the canaliculus. This description of time-dependent spatial mineralization patterns, will allow the interpretation of known mineralization disorders in the context of our model.

Advanced materials and smart structures: Modeling, simulation and testing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DESIGN AND MULTISCALE ANALYSIS OF AN ARCHITECTED MATERIAL WITH VOLUMETRIC ELASTIC PHASE TRANSITIONS

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ABSTRACT

Materials characterized by non-quasiconvex strain energies experiment microscale phase transitions when the strain state switches between different convex regions of the energy landscape. This type of phase transition offers a range of notable features, within which the repetitive energy release is of special interest for potential use in reusable energy dampers. It is well-known that non-quasiconvexity of the energy causes that, when the equilibrium of bodies composed by this kind of materials is resolved, it is possible to guarantee, in general, neither uniqueness nor existence. Additionally, the relaxation/quasiconvexification of the strain energies generates a closely related problem that is, contrarily, well-posed. This work exploits these concepts to address a comprehensive multiscale study of mechanical metamaterials with microscale elastic phase transitions. The emphasis is on phase transitions between two strain energy wells separated along volumetric strains, facilitating realistic applications in multidirectional energy release. At the macroscale, a generalized standard material model is proposed, defined through an energy potential and a dissipation potential. Both potentials derive from appropriate average calculations of microscale counterparts. In this sense, the relaxation of the microscale non-quasiconvex strain energy serves as the energy potential (see [1]), while the dissipation potential is obtained by homogenizing the microscale released energy. This methodology enables the examination of macroscopic hysteresis, in closed cycles of stress-strain responses when energy barriers of the energy landscape are not automatically surpassed, and the corresponding microstructure formation (highly oscillating strain fields). Numerical results are compared with theoretical estimations provided by [2]. The microarchitecture design of a 3D metamaterial capable of achieving volumetric phase transitions is also proposed. The metamaterial phase transitions result from elastic instabilities due to a geometrically non-linear deformation within the elastic range of the constituent material. The presented novel design builds upon microarchitectures previously introduced by [3] and extends them to three dimensions.

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Advances in numerical methods for solution of PDEs
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A FRACTIONAL FINITE ELEMENT FORMULATION FOR BENDING ANALYSIS OF VISCOELASTIC PROBLEMS

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ABSTRACT

This article introduces a novel fractional finite element approach for the precise modeling of viscoelastic behavior in one-dimensional (rod) and two-dimensional (plane) problems. The viscoelastic properties of the material are represented using the fractional Kelvin-Voigt model, employing a combination of spring and fractional dashpot elements. While the fractional viscoelastic model demonstrates enhanced solution accuracy compared to conventional viscoelastic models, accurately defining the fractional derivative remains a challenge. To address this, a Gaussian Jacobi quadrature numerical method is integrated into the finite element formulation for calculating the fractional derivative of the fractional dashpot within the range of zero to one. The finite element discretization algorithm employs a polynomial Jacobi approach for computing the stiffness matrix and viscous loading. Notably, a recursive formulation updates the data at the end of each time increment, ensuring computational efficiency. A key advantage of this method is the reduced need for Gaussian points, leading to faster solutions and improved computational efficiency. The proposed model is validated against classical models to demonstrate its accuracy and precision.

Keywords: Viscoelastic material, Fractional derivative, Finite element method, Kelvin-Voigt model.

Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING BRITTLE FRACTURE IN EPOXY POLYMERS USING ATOMISTIC-CONTINUUM COUPLING OF MD WITH FEM

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ABSTRACT

The prediction of brittle fracture properties in polymeric materials using atomistic simulations is still a challenge. One of the main challenges is that the crack size in epoxy needs to be greater than 2590 nm to display full notch sensitivity, and that the fully developed fracture process zone size needs to be modeled contained within a zone of K-dominance. Consequently, , due to the intense computational cost of running atomistic simulations, the range of crack lengths simulated has been severely limited. In this work, we use the state-of-the-art multiscale modelling techniques to allow atomistic simulations to run with much larger crack lengths and study the effect of crack length variation on failure behavior. A thermosetting epoxy polymer system of EPON862/DETDA is modelled using the ReaxFF molecular dynamics (MD) force field, which allows for bond breakage. The MD system is concurrently coupled with a much larger continuum system modelled by the finite element method (FEM). The atomistic-continuum coupling is performed using a novel anchor-point based statistical method incorporating internal volume cells (IVCs), with displacement and strain continuity enforced in the handshake region using Lagrange multipliers. The combined system is used to simulate a double cantilever beam (DCB) specimen, with the MD domain surrounding the crack tip to capture nanoscale bond breakage. The critical strain energy release rate (SERR) is computed using the atomistic J-integral specifically developed by the authors for simulating fracture in amorphous polymers. The crack length of the system is varied and its effect on the SERR is studied. The atomistic J-integral contour is designed to include the crack tip in the MD region but can be allowed to extend well into the handshake region, if deemed necessary. The open-source LAMMPS code is used to run MD simulations at a finite temperature. The linear elastic in-house FEM code is integrated into an in-house concurrent coupling code, which iteratively executes the coupled MD simulations using a staggered solution scheme. Benchmarking of the code was carried out by simulating brittle fracture in monocrystalline graphene sheet. Our preliminary results for epoxy indicate a monotonic increase in notch-sensitivity with increasing subcritical crack length.

Model order reduction for parametrized continuum mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

REDUCED ORDER MODELLING IN CFD: GEOMETRY, TURBULENCE AND COMPRESSIBILITY ENHANCED BY SCIENTIFIC MACHINE LEARNING

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ABSTRACT

We focus on some perspectives about Reduced Order Methods (ROM) for parametric Partial Differential Equations (PDEs) with a special interest in parametric problems arising in offline-online Computational Fluid Dynamics (CFD), with a special attention to the enhancement provided by Scientific Machine Learning (SML). Efficient parametrisations (random inputs, geometry, physics) are very important to be able to properly address an offline-online decoupling of the computational procedures and to allow competitive computational performances. Current ROM developments in CFD include: (i) a better use of stable high fidelity methods, to enhance the quality of the reduced model too, also in presence of bifurcations and loss of uniqueness of the solution itself, (ii) capability to incorporate turbulence models and to increase the Reynolds number; (iii) more efficient sampling techniques to reduce the number of the basis functions, retained as snapshots, as well as the dimension of online systems; (iv) the improvements of the certification of accuracy, established on residual based error bounds, and of the stability factors, as well as (v) the guarantee of the stability of the approximation with proper space enrichments. All the previous aspects are quite relevant -- and often challenging -- in CFD problems to focus on real time simulations for complex parametric industrial, environmental and biomedical flow problems, or even in a control flow setting with data assimilation and uncertainty quantification. Some model problems will be illustrated by focusing on few benchmark study cases, for example on simple fluid-structure interaction problems and on shape optimisation, applied to some industrial and environmental problems of interest.

Battery modeling and computation: From material to device
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THEORETICAL UNDERSTANDING OF CRITICAL ISSUES IN ALL-SOLID-STATE BATTERIES: SINTERING, CRACKING, AND DENDRITE PENETRATION

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ABSTRACT

All-solid-state lithium metal batteries (ASSLMBs) are considered to be the most promising next-generation batteries because of their perceived electrochemical, mechanical, and thermal stability. The existing problems hindering their way to commercialization are the cracking of solid electrolytes (SEs) and cathodes and the penetration of dendrites. These issues are difficult to solve based soley on experiments and electro-chemo-mechanical Multiphysics models can set in to provide details bridging the fragmented experimental observations. This presentation introduced several ongoing endeavors in theoretical models. For the lithium penetration through SEs, we proposed a phase-field (PF) model to describe interfacial defects caused by electro-stripping, SSE cracking caused by chemical expansion/contraction during ion transport, and lithium penetration caused by an inhomogeneous electric field. With the model, we reveal the critical current density (CCD) and how it depends on material parameters. Additionally, it is found that the residual compressive stress at SE surfaces can effectively prevent SSE cracking. Using the PF formulations, we then studied glass fracture after a residual stress field is developed by the ion exchange, which may also be applied to strengthen SEs. A dense SE provides a compact surface in contact with an Li anode and it can lead to a small interfacial resistance with less interfacial defects for crack initiation. Nevertheless, SEs, e.g., LLZTO, after sintering at atmospheric pressure are likely porous due to decomposition and Li escape. Hence, a PF model of LLZTO sintering can be built to quantitatively investigate the competition between Li escape and LLZTO particle coalesce for optimizing the temperature profile to sinter dense LLZTO. Finally, we discussed the possible way to toughen NCM cathodes, of which the volumetric changes during lithiation and de-lithiation lead to catastrophic fatigue fracture. Based on a theoretical model, we argue that introducing soft polymeric interlayers between partially sintered NCM particles can improve the cyclic performance of NCM cathodes.

ROBUST VIRTUAL ELEMENT METHODS FOR STRESS-ASSISTED DIFFUSION PROBLEMS

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ABSTRACT

This paper aims first to perform robust continuous analysis of a mixed nonlinear formulation for stress-assisted diffusion of a solute that interacts with an elastic material, and second to propose and analyse a virtual element formulation of the model problem. The two-way coupling mechanisms between the Herrmann formulation for linear elasticity and the reaction-diffusion equation (written in mixed form) consist of diffusion-induced active stress and stress-dependent diffusion. The two sub-problems are analysed using the extended Babuˇska–Brezzi–Braess theory for perturbed saddle-point problems. The well-posedness of the nonlinearly coupled system is established using a Banach fixed-point strategy and an assumption on small data. The virtual element formulations for the uncoupled sub-problems are proven uniquely solvable by a fixed-point argument, now in conjunction with appropriate projection operators. A priori error estimates are derived, and we test the accuracy and performance of the proposed method through computational simulations.

Multiphysics and data-driven modeling for cardiovascular biomedicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN PREDICTION OF REDUCED-ORDER CARDIOVASCULAR MODEL PARAMETERS

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ABSTRACT

Cardiovascular flow simulations have become a powerful tool for the study and management of cardiovascular in recent decades. They provide insight into the hemodynamic characteristics of diseased anatomies and the mechanisms by which they develop, aid in surgical planning by predicting the hemodynamic outcomes associated with proposed anatomical modifications, and support the development of medical devices. Unfortunately, traditional, high-fidelity finite element flow simulations that solve the unsteady Navier-Stokes equations in three dimensions (3D) are computationally expensive. This limits their use in many settings, including clinical applications, multi-query applications, and real-time simulators. In these use cases, reduced-order models (ROMs) that resolve the flow associated with simplified, but analogous systems are attractive alternatives to 3D simulations.

In this work, we focus on a popular zero-dimensional (0D) model in which the vasculature is represented as an idealized electric circuit where flow and pressure are analogous to current and voltage, respectively. Although computationally lightweight, the 0D ROM suffers from reduced accuracy due, in part, to the imperfect translation of the 3D flow problem into its 0D analog. To express a 3D vasculature as a 0D model, the vasculature is divided into vascular components (vessels and junctions), each of which is represented by an ideal wire populated with circuit elements (e.g. linear resistors, quadratic resistors, inductors) that describe the relationship between flow through the component and the pressure drop over the component. Traditionally, the characteristic values of these circuit elements are chosen based on the geometry using physics-based models that rely on simplifying assumptions that may not apply or heuristic techniques.
We propose data-driven techniques to construct improved 0D representations of vascular components. Specifically, we develop machine learning (ML) models that take the geometric features of the vasculature component as input and output characteristic values of the electric circuit elements. To construct datasets on which to train and test our models, we use an automated workflow in which we generate junction geometries, run a series of 3D flow simulations on each geometry, and extract the characteristic circuit element values for each geometry from its 3D simulation (ground truth) data. By supplying more accurate characteristic circuit element values to the 0D model, we improve its ability to model cardiovascular flows.

Advanced discretization schemes and solution strategies for computational structural dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN EXPLICIT TIME-MARCHING PROCEDURE FOR ELASTODYNAMIC ANALYSES BASED ON ADAPTIVE TIME-INTEGRATION PARAMETERS AND TIME-STEP VALUES

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ABSTRACT

This study discusses an explicit time-marching procedure that is designed for the time-domain resolution of elastodynamic models considering their physical properties and adopted spatial discretizations. The technique is entirely automated and proves itself to be highly effective, featuring second-order accuracy, adaptive algorithmic dissipation and extended stability limits. Additionally, the discussed methodology is truly explicit, truly self-starting, and it incorporates automated subdomain/sub-cycling splitting procedures to enhance its overall performance. Thus, the algorithm automatically divides the domain of the problem into different subdomains, adjusting their time-step values according to the properties of the discretized model, which allows improving the efficiency and the accuracy of the analysis, while ensuring stability. Locally-defined adaptive time-integration parameters are also considered, establishing an entirely self-adjustable formulation. In this case, expressions for the time-integration parameters are provided based on the local features of the discrete model, allowing to create a further link between the adopted temporal and spatial discretization procedures, better counterbalancing their errors. These parameters are locally formulated to nullify the bifurcation spectral radius of the method at pre-established sampling frequencies, providing maximal numerical damping at the highest sampling frequency of the elements of the adopted spatial discretization. This design optimizes the formulation to mitigate the influence of spurious high-frequency modes on the computed responses, allowing for enhanced analyses. In fact, the primary goal of introducing numerical damping is to eliminate non-physical spurious oscillations that may arise from the excitation of spatially unresolved modes. Therefore, the methodology not only tracks down the frequency range of the discretized model, but also it is designed to adaptively enforce significantly low values (close to zero) for the spectral radius of the method at the highest frequencies of the model, as well as it aims to provide relatively high spectral radius values (close to one, considering physically undamped models) in the important low-frequency range. Benchmark analyses are conducted at the end of this study to demonstrate the technique's effectiveness taking into account theoretical problems and complex models that are representative of real-world applications in the OIL & GAS industry.

Next-generation numerical methods for coupled multiphysics problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FULLY MIXED FORMULATIONS FOR POROELASTICITY WITH STRESS-DEPENDENT PERMEABILITY

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ABSTRACT

We use fixed-point arguments to analyse the unique solvability of a nonlinear system of PDEs modelling poroelasticity equations with porosity-dependent permeability. The permeability is rewritten as a function of total poroelastic stress and fluid pressure. We construct fully mixed finite element methods and show their optimal convergence to weak solutions. A priori and a posteriori error bounds are established. Some numerical examples are provided to confirm the rates of convergence predicted by the theory, and we also illustrate the use of the formulation in some typical tests in Biot poroelasticity.

Multiphysics and data-driven modeling for cardiovascular biomedicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SIMULATING PULSATILE FLOW: TOWARDS UNDERSTANDING MICROVASCULAR DYSFUNCTION

Hans Christian Rundfeldt[1], Mario Gilberto Báez-Yáñez[1], Jaco Zwanenburg[1] and Natalia Petridou[1]*

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ABSTRACT

Pulsatile flow and pressure provide a proxy for vascular health. Increased pulsatility due to vascular stiffening is observed in different pathologies of the cerebrovascular system [1]. Pulsatility in larger vessels can be assessed in-vivo by medical imaging. In the microvasculature, pulsatility can only be assessed indirectly using functional MRI acquisitions [2]. However, the formation of MRI signal based on the underlying microvasculature and tissue remains elusive due to voxel-averaging, limiting the ability to investigate changes and dysfunction of small vessels severely.

To address this problem, we propose the generation of statistically informed microvascular models at the voxel level. These are used to simulate dynamic pulsatile blood flow and pressure changes in small arterioles, capillaries, and venules. A synthetic tree generation algorithm was utilized to generate two-dimensional realistic microvasculature covering an area of 3500x3500µm. The generated vasculature extends from the pial surface over six cortical layers to the gray-white-matter boundary. Penetrating arteries and veins are generated to varying depths. Capillary structures were generated using random bifurcations defined by a Delaunay triangulation. The statistical properties of the networks were matched to rodent data [3] and Murray’s law was enforced throughout the network. A 1D non-linear approximation of the Navier-Stokes equations is used to describe blood flow. The vessel wall deformation is assumed as purely elastic. Fluid-structure interaction is considered by coupling the computed blood pressure and wall deformations using a constitutive tube law. The governing equations were solved using a custom finite volume implementation. We conducted a sensitivity study of the model parameters, simulating the impact of vascular stiffening and changes in wall thickness on the pulsatility.

This work opens up the possibility to investigate pathologies that manifest themselves predominantly in the microvasculature such as small vessel disease and cerebral amyloid angiopathy (CAA). The simulated vessel pulsatility will be compared to fMRI data from diseased patients and healthy controls to further assess the validity of this approach.

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Modern structure-preserving methods for PDEs
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SCALABLE OPTIMAL CONTROL FOR INEQUALITY-CONSTRAINED DISCRETIZATIONS OF CONSERVATION LAWS

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ABSTRACT

A physically meaningful solution of a conservation equation has to satisfy certain constraints such as the validity of global maximum principles or the conservation of mass. If the analytical solution of the problem is bound preserving, closed-form limiters can be used to enforce appropriate inequality constraints for numerical approximations. However, if modeling errors or data errors are present, even exact solutions may violate global bounds that define the range of physically admissible approximations. To avoid such nonphysical behavior, we incorporate optimal control into discretized conservation laws. Following the methodology developed in [1], we consider inequality-constrained optimization problems in which the desired properties are enforced using graph Laplacian operators and flux potentials. The objective function penalizes deviations from nodal time derivatives corresponding to a high-order space discretization. The adjustable source term of the PDE constraint admits a decomposition into numerical fluxes, which enables us to achieve good local mass conservation properties.

In this presentation, we outline the derivation of the optimization problem and its connection to the optimization-based approaches developed in [2]. A potential drawback of formulations that use flux potentials as optimization variables is the lack of scalability for large-scale simulations. To develop an efficient alternative, we reformulate our optimization problem in terms of control variables from which flux potentials can be recovered by solving a linear system. The result is a quadratic optimization problem with box constraints and a linear equality constraint. For the corresponding system of optimality conditions, we use scalable trust-region solvers and scaling operators that serve as simple preconditioners. Besides, we discuss different choices of norms and seminorms for the objective function, as well as their influence on the convergence behavior. Further improvement is achieved by using multigrid preconditioning and inexact evaluations of objective, gradient and Hessian functions. To illustrate the viability of our new method, we present results for a linear advection problem (solid body rotation in 2D) and for the Cahn-Hilliard equation (merging droplets and spinodal decomposition in 3D).

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Modeling and simulation of the electro-chemo-thermo-mechanical interactions in energy transition and energy storage systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELLING AND SIMULATION OF A FULLY ELECTRIC HYBRID PROPULSION SYSTEM FOR PASSENGER SHIPS USING AVL CRUISE-M SOFTWARE

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ABSTRACT

The design and performance optimization of fully electric ships constitutes an integral goal of the maritime sector to meet the emission requirements and comply with the IMO environmental regulations.
Hybrid powertrains integrating fuel cell technology with energy storage systems are spreading worldwide in transportation. This research uses the AVL Cruise-M software to validate a PEM fuel cell power generation system integrated with a Li-based battery and the onboard propulsion mechanism. The proposed powertrain architecture and operating modes' working principles are presented from a system engineering perspective. The specifics of each component of the power train (e.g. the PEMFC module and its BoP, the battery pack, the electric motor, etc.) are taken from commercially available products.
As the scope of simulations, the ship's operating modes are tested over a predefined cruise cycle which is also used to size the power of each component and predict the fuel consumption. The objective is to assess the dynamic functionality of such a system and analyze the energy flows, including the corresponding Balance of Plant (BoP) subsystems. The cruise cycle is meant as a round trip lasting approximately 6.5 hours, with 44% of the total time spent in transfer mode at full speed, 35% in laytime, and the remaining 21% in maneuvering.
As a case study, we assume a passenger ferry with dimensions of approximately 30 meters in length and 10 meters in width. The ferry has a passenger capacity of 220 and a maximum cruise speed of 20 knots. The simulation results show that a PEM system with a maximum power of 1600 kWe can fulfil the ship's power demand, while a battery pack of about 200 kWh can support the PEM system during dynamic conditions, particularly during forceful accelerations. This enhances the ship's performance and increases the overall energy efficiency.
Considering the available space on board and the fuel consumption per cruise cycle, it is supposed to store about 350 kg of pure hydrogen in type IV cylinder tanks at 700 bars, which can be refilled daily.

Data science and machine learning applications for composite materials and biomedical engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MACHINE LEARNING-DRIVEN OPTIMIZATION OF 3D PRINTING COMPOSITE STRUCTURES AND PROCESSES

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ABSTRACT

This presentation delves into the strategic application of artificial intelligence (AI) to enhance the capabilities and processes of 3D printing, illustrated through two distinct case studies. Initially, we present a data-driven design methodology that focuses on refining bio-inspired composite materials with a limited dataset. This approach results in an optimized set of composite designs that adeptly combine strength, durability, and lightweight characteristics. In the latter part, we introduce a simulation model for the Digital Light Processing (DLP) 3D printing method, which is pivotal in managing the residual stresses that emerge from the process. This model is key to foreseeing and mitigating unwanted warping in 3D printed objects following DLP printing. By integrating this simulation with real-world data in a data-optimized strategy, we showcase how to attain the desired structure with minimal distortion.

New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PEM FUEL CELL TOPOLOGY OPTIMIZATION WITH A PSEUDO 3D MODEL

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[1]*University of São Paulo*

ABSTRACT

The research related to clean energy sources is a growing topic nowadays. This work focuses on optimizing a hydrogen proton exchange membrane fuel cell to increase electric power generation. The model considers a pseudo-3d model to reduce the computational cost of the highly multi-physics problem across all cell layers. The model includes navier-stokes, energy conservation, chemical species transport, and water transport equations. The system is solved using a finite element formulation, and the sensitivities are calculated via automatic derivation. The optimization consists of a multi-objective function combining power generation and current density homogenization. An interior point gradient-based optimizer is used. The results show simultaneous optimized topologies for the cathode and anode flow fields.

Advanced computational modelling of wood, wood-based products, bio-composites, and timber structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ROLLING SHEAR SIMULATIONS IN CROSS LAMINATED TIMBER STRUCTURES USING A DOMAIN DECOMPOSITION METHOD

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ABSTRACT

Cross-Laminated Timber (CLT) is an engineered-wood product made of stacked lumber boards; each layer is usually oriented perpendicular to others and glued with structural adhesives. CLT are being increasingly used as structural materials due to environmental reasons and because of their remarkable mechanical strength. However, when designing CLT boards, the study of cracking propagation still requires further investigation due to the so-called rolling-shear failure [1] which is the inter-fiber cracking due to shear strains in the plane perpendicular to the longitudinal axis of the wood fibers. Indeed, the shear stiffness between radial and tangential directions is two hundred times lower than the stiffness in fibers' direction. The buckling of CLT walls is another important scenario – especially in mid-rise CLT building – where a weak rolling-shear strength could induce the apparition of cracks in cross layers. The combination of such anisotropy with thick sections is relatively new in the field of composite materials.

This work focuses on simulating the non-linear behavior of CLT structures using a computational strategy based on a mixed domain decomposition method [2]. We propose the integration of damage models at different scales (i.e. delamination between layers and crack propagation inside the layers) using cohesive zone models and parallel computing. Preliminary results show the beginning and spread of cracks in rolling-shear failure; the influence of the structural adhesive stiffness on the critical buckling load of the CLT walls is also analyzed [3]. Additionally, cohesive zone models – a bilinear, a trilinear and a potential one – are characterized using the equivalent linear elastic fracture mechanics (LEFM) R-curve. Such numerical-experimental methodology is studied considering double cantilever beam (DCB) tests performed in Chilean radiata pine specimens.

ACKNOWLEDGEMENTS
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Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MINIMAL REMESHING VEM TECHNIQUE FOR COHESIVE FRACTURE NUCLEATION AND GROWTH

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ABSTRACT

Recently, the virtual element method (VEM) has strongly developed and has proved to cope with a wide range of topics and problems. In particular, VEMs can be conveniently applied to the computational fracture mechanics applications.

The VEM formulation is characterized by the possibility to define polygonal meshes with elements characterized by any number of edges and by the flexibility in mesh generation that allow to introduce a crack just splitting the element in two different elements joined by a crack modelled with an interface element, requiring a minimal remeshing.

The present work proposes an algorithm for the nucleation and growth for fracture evolution in 2D cohesive media. The procedure is based on an enhanced virtual element method [1] specifically referred to a 4-side 12-node virtual element with piece-wise linear approximation of the displacement field on the edges. The large number of nodes and, consequently of degrees of freedom, is exploited to enrich the strain field evaluation. The proposed approach is framed within a generalization of the classic VEM formulation, obtained by introducing an energy norm in the projection operator definition. Various enhancements are proposed and tested through several numerical examples. The proposed procedures allow to avoid the stabilization of the element stiffness matrix.

Moreover a numerical technique is considered in order to introduce the crack in one virtual element splitting it in two elements joined by a cohesive interface [2]. An interface cohesive law, introducing a damage variable in mode I, in mode II and in mixed mode, and taking into account the unilateral effect due to the reclosure of the fracture in compression, is adopted.

Finally, different procedures are considered in order to evaluate the crack-tip stress field and the crack propagation direction.
The mixed-mode fracture examples are developed in order to assess the ability of the proposed procedure to satisfactorily reproduce the crack nucleation and growth observed in experimental tests.

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Advances in computational biomechanics and mechanobiology
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FRACTIONAL DARCY'S LAW FOR POROELASTIC BEHAVIOUR OF SOFT BIOLOGICAL TISSUES: APPLICATION TO MENISCUS

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ABSTRACT

The meniscus is an important part of the knee joint that helps with lubrication and shock absorption. Its porous structure and the flow of fluid through its pores are crucial for its functionality. Usually, poroelasticity is used to study this behaviour, which assumes Darcian flow. However, in reality, the fluid undergoes anomalous diffusion, which is non-Darcian [1]. To study this behaviour in the meniscus, researchers have used fractional Darcy's law for poroelasticity [2]. Confined consolidation creep experiments were conducted on the meniscus tissue to obtain its material properties, and the model was validated using stress relaxation tests and weight loss during consolidation. Results show that the fractional Darcy's law works better than the traditional one. Experimental data from different regions and orientations were used to study the anisotropic and inhomogeneous nature of the meniscus. The meniscus can be treated as a transversely isotropic poroelastic material, and its permeability is higher in the circumferential direction compared to the radial and vertical directions. A 3D fractional poroelastic model was implemented in 'Abaqus software [3], and simulations were performed on the whole meniscus, considering its functionally graded nature. The simulations studied quantities such as the flux of interstitial fluid during the consolidation process and energy absorption.

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Computational modeling of cardiac fibrosis: A multiscale, multiphysics challenge
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A HIGH-FIDELITY 3D MICROMECHANICAL MODEL OF VENTRICULAR MYOCARDIUM

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ABSTRACT

Right ventricular (RV) failure in response to pulmonary hypertension (PH) is a severe disease that remains poorly understood. PH-induced pressure overload leads to changes in the RV free wall (RVFW) that eventually results in RV failure. While the development of computational models can benefit our understanding of the onset and progression of PH-induced pressure overload, detailed knowledge of the underlying structural and biomechanical events remains limited, especially in the onset and progression of fibrosis in the RVFW. We have previously demonstrated the importance of myofiber-collagen mechanical interactions in modeling the passive mechanical behavior of right ventricle free wall (RVFW) myocardium. To gain deeper insights into these coupling mechanisms, we developed a high-fidelity, micro-anatomically realistic 3D finite element model of right ventricle free wall (RVFW) myocardium by combining high-resolution imaging and supercomputer-based simulations. We first developed a representative tissue element (RTE) model at the sub-tissue scale by specializing the hyperelastic anisotropic structurally-based constitutive relations for myofibers and ECM collagen, and equi-biaxial and non-equibiaxial loading conditions were simulated using the open-source software FEniCS to compute the effective stress-strain response of the RTE. To estimate the model parameters of the RTE model, we first fitted a 'top-down' biaxial stress-strain behavior with our previous structurally based (tissue-scale) model, informed by the measured myofiber and collagen fiber composition and orientation distributions. Next, we employed a multi-scale approach to determine the tissue-level (5 x 5 x 0.7 mm specimen size) RVFW biaxial behavior via 'bottom-up' homogenization of the fitted RTE model, recapitulating the histologically measured myofiber and collagen orientation to the biaxial mechanical data. Our homogenization approach successfully reproduced the tissue-level mechanical behavior of our previous studies in all biaxial deformation modes, suggesting that the 3D micro-anatomical arrangement of myofibers and ECM collagen is indeed a primary mechanism driving myofiber-collagen interactions. Through this approach, we determine that the interactions occurring at the tissue scale can be accounted for by accurately representing the geometry of the myofiber-collagen arrangement at the micro scale. Ultimately, models such as these can be used to link cellular-level adaptations with organ-level adaptations to lead to the development of patient-specific treatments for PAH.

Advances in computational biomechanics and mechanobiology
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AORTIC STENOSIS AND MYOCARDIAL REMODELING: INSIGHTS FROM FINITE ELEMENT ANALYSIS IN A RAT MODEL

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ABSTRACT

Aortic stenosis (AS) is a prevalent valvular heart disease characterized by the narrowing of the aortic valve, leading to increased cardiac afterload and myocardial remodeling. AS is also a common cause of heart failure with preserved ejection fraction (HFpEF), a condition where heart failure symptoms occur despite normal ejection fraction (EF) [1]. This condition undermines the effectiveness of conventional diagnostic measurements such as EF and global longitudinal strain (GLS) [2]. This study aims to use finite element analysis to investigate the alterations in myocardial mechanical behavior under the influence of AS and assess the diagnostic performance of myocardial work (MW) as an emerging index.

We utilized datasets from a rat model of increased afterload via aortic banding. Rat samples were subjected to three levels of constriction of the ascending aorta using o-rings with fixed inner diameters, ensuring precise aortic constriction [3]. This simulates aortic stenosis, leading to ventricular hypertrophy and myocardial remodeling. Additionally, a sham experiment was conducted to establish a control group. MRI was performed longitudinally on each group at two, four, eight, and twenty weeks post-operation. MR images were then used to create subject-specific geometries at end diastole. Employing the measured pressure-volume curves during the experiment, finite element (FE) models were created and tuned to estimate the passive and active material behavior of the myocardium throughout the development of induced AS and MW for each segment of the left ventricle calculated from the FE models.

FE models provide insights into the time-dependent mechanical remodeling of myocardial tissue due to increased afterload. Importantly, this research evaluates the potential of FE-based MW as an advanced metric for diagnosing HFpEF in cases of AS. While MW has been previously utilized based on echocardiography, these methods do not account for thickness, or curvature, all of which can be altered in the presence of abnormal afterload [1].

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Biomechanics of hard tissues: From experiments and simulations to clinical applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL INVESTIGATION INTO THE HYGRO-MECHANICAL RESPONSE OF SWELLING IMPLANTS AND THE BONE REMODELING AROUND THEM

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ABSTRACT

In this study, a hygro-elastic finite element framework, along with a strain-energy-density based bone remodeling framework, were developed and used to simulate the swelling of co-polymeric implants and bone anchors in order to investigate their hygro-mechanical response [1, 2]. Free swelling experiments were conducted on co-polymeric porous bone anchors (composed of cross-linked poly (MMA-AA)) with two ratios of 80/20 and 90/10, to investigate their swelling characteristics in bovine serum, mimicking the in-vivo conditions. The purpose for the use of the two compositions is to have means of comparison and to analyze the optimal swelling ratio. Using the free swelling experimental data (i.e., weight gain and dimensional changes), the hygro-elastic framework was validated. Subsequently, the swelling of bone anchors was simulated embedded in bone regions with different densities. The radial stresses induced in the interface were extracted to ensure the sensible fixation strength of the bone anchor, as well as to look into the mechanical response of the surrounding bone and the associated bone regeneration. According to Wolff's law, such mechanical loads can be regarded by bone mechanotransducers as stimuli for remodeling [3]. Therefore, the bone remodeling framework helped us to evaluate the impact of the radial force induced by the swelling on the surrounding bone. It was discovered that the swelling ratio plays an important role in bone remodeling, and that it must be controlled within a certain threshold.

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Mesh-free particle methods for multi-physics problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN INCOMPRESSIBLE SPH STRATEGY FOR MULTI-PHYSICS' INTERFACIAL PROBLEMS

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ABSTRACT

In this work, we investigate the synergistic impact of electro-hydrodynamic (EHD) and thermo-capillary (TC) forces on the dynamic behaviour of multiphase flow systems. The study employs an incompressible Smoothed Particle Hydrodynamic (ISPH) multiphase model to simulate flows driven by EHD and TC forces. To capture the intricate hydrodynamic interactions, the continuum surface force (CSF) method is employed. This method calculates the gradient of interfacial tension and Marangoni forces, achieving an approximate error of less than 0.02% in Marangoni force calculations compared to analytical solutions. This represents a substantial improvement over previous SPH simulation studies.
EHD phenomena integrated into the system by solving the Maxwell stress tensor. It also influence interface morphology based on the electrical characteristics the surrounding fluids, i.e. electrical permittivities and conductivities. We study diverse test cases and integrates novel benchmarks. These encompass the EHD deformation of a droplet within a fluid, interactions of multiple droplets, and the Rayleigh-Taylor instability in the presence of an external electric field. The findings presented herein demonstrate the remarkable efficacy of the proposed SPH method and its resilience in simulating multiphase flows characterised by intricate interfaces when subjected to a consistent external electric field as well as thermal stresses.

ACCELERATING PHASE FIELD SIMULATIONS THROUGH TIME EXTRAPOLATION USING NEURAL OPERATORS AND GENERATIVE MODELS

Cosmin Safta[*1], Christophe Bonneville[1], Arun Hegde[1], Habib Najm[1] and Laurent Capolungo[2]*

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ABSTRACT

Computational simulation of phase field dynamics can be prohibitively expensive when using standard numerical solvers. For example, high-fidelity simulations often use very small time steps due to stability considerations, which can become a bottleneck when the target quantities of interest require predictions far out in time. To address this challenge, we employ machine learning-based surrogate models to help extrapolate forward in time, enabling predictions at time horizons far beyond what is achievable through traditional methods alone. Specifically, we investigate two deep learning architectures, Fourier Neural Operators (FNOs) and UNets, and train them to predict future states with much coarser time steps – thus encapsulating multiple high-fidelity steps within a single surrogate evaluation. While this approach enables more rapid predictions through autoregressive evaluation of the surrogate, the incurred error is essentially uncontrolled. To alleviate this, we adopt a hybrid prediction strategy which alternates between surrogate evaluations – which leap forward in time – and high fidelity simulation steps – which reduce errors and bring the system state back to the solution manifold. Moreover, we show that including periodic retraining using synthetic data obtained via diffusion models can improve the quality of the surrogate models. We illustrate these methods on two examples, a simpler Cahn-Hilliard system and a more sophisticated liquid metal dealloying simulation.

Advances in damage & fracture modeling of multiphysics materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

REPRESENTATIVE VOLUME ELEMENT MODEL FOR PREDICTING THE COBLE CREEP DEFORMATION AND VOID NUCLEATION/GROWTH IN THREE-DIMENSIONAL POLYCRYSTALLINE STRUCTURE

Kota Sagara[*1] and Kazuki Shibanuma*[1]

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ABSTRACT

A model is proposed to quantitatively predict the Coble creep deformation and void nucleation/growth in a three-dimensional polycrystalline. The model is developed for a three-dimensional representative volume element containing multiple grains to predict the effects of three-dimensional polycrystalline morphology. The proposed model consists of a creep deformation model and a void nucleation/growth model.
The creep deformation model comprises both static grain growth and dynamic grain growth. Static grain growth is driven by the movement of grain boundary in a direction that reduces the total grain boundary energy. Dynamic grain growth is induced by the diffusion flux on grain boundary, and the growth rate is calculated by relative velocity of grain boundary, which is the rate at which the thickness of grain boundary changes.
Distinct models are developed for the process of void nucleation and growth. The void nucleation probability is calculated by the relative velocity of grain boundary, and voids are randomly generated on grain boundary. The size of the nucleated void is determined based on the conditions for the stable existence of void on grain boundary derived from Helmholtz's free energy. Void growth is carried out in two separate stages. First, each void grows in the direction of grain boundary. The volume change during this stage is determined by the summation of the volumetric diffusion flux of atoms flowing from the voids to the grain boundary. Next, by calculating the diffusion flux on the surface of each void, void grows in the direction perpendicular to the grain boundary. Throughout this process, the volume of the void is kept unchanged.
The developed model was validated by comparing with the theoretical formula of Coble creep and tendency of experiments. Also, the model was able to evaluate the effects of factors that could not be taken into account in the conventional theoretical equations. Consequently, this study has established the foundation for a model to quantitatively predict the deformation and void nucleation/growth caused by Coble creep.

Data-driven approaches for solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEEP LEARNING BASED ACCELERATED HIGH STRAIN RATE SIMULATIONS FOR DESIGN OF MATERIALS IN EXTREME ENVIRONMENTS

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ABSTRACT

Designing materials with the desired mechanical properties using a combinatorial approach often necessitates multiple iterations. The expense of conducting experiments in each iteration to ascertain material properties can be exorbitantly high. An alternative is leveraging computational models. However, executing high-fidelity, physics-based simulations can be time-consuming. A faster method involves employing deep learning (DL) based models as surrogate models to predict desired parameters. Our current research focuses on laser-driven spall experiments conducted on thin foils. These laser-driven spall tests are high-strain rate experiments (approximately 10^6). They are instrumental in determining the spall strength of materials. Our goal is to develop DL-based techniques to predict spall strength and other relevant parameters from given microstructures. To this end, we will use data from crystal plasticity finite element simulations as the baseline for our analysis.

Enabling technologies for digital twins: Model reduction and scientific machine learning
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ENGINEERING SOFTWARE 2.0 FOR DIGITAL TWIN: UNIFICATION OF TRAINING, CALIBRATING, AND LEARNING THROUGH KERNEL INTERPRETATION OF NEURAL NETWORKS

Sourav Saha[*1] and Wing Kam Liu*[1]

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ABSTRACT

The field of computational mechanics is evolving from software 1.0, with explicit, task-specific programming, to software 2.0, which uses data and optimization. However, a direct transition to software 2.0 is extremely difficult for engineering science because a) data is scarce for many engineering systems, b) modeling complex multiphysics problems requires extensive calibration of parameters, and c) augmenting the experimental data with the computational model is extremely time-consuming. Consequently, we should focus on Engineering Software 2.0 which is an end-to-end software system that unifies solving, calibrating, and training in science, engineering, and manufacturing problems. Engineering Software 2.0 defines all problems in optimization construct and leverages automatic differentiation to solve unknown parameters. A gap exists in the contemporary computational and/or theoretical methods that can engender engineering software 2.0. This talk explores the connection between kernel methods in machine learning and deep neural networks, demonstrating how this perspective bridges the gap between interpolation methods in numerical analysis and the concept of universal approximation in neural networks. The presentation is built upon the mathematical foundations of Deep Learning Discrete Calculus (DLDC) [1] and the scientific and engineering principles of Hierarchical Deep Learning Neural Network (HiDeNN) [2], and will show how to solve three general types of problems encountered in science and engineering with this new approach. The first type of problem occurs when there is no known closed-form physical equation. The second type arises when the knowledge of governing laws is incomplete. Lastly, the third type of problem involves known governing equations where computational speed needs improvement. All these three types of problems are to be solved in unified engineering software 2.0. The talk will present a demonstration of this software system and shed light on how it works.

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Constitutive modeling of complex materials with machine learning and artificial intelligence
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GENERATIVE HYPERELASTICITY WITH PHYSICS-INFORMED PROBABILISTIC DIFFUSION FIELDS

Francisco Sahli Costabal[*1], Vahidullah Taç[2], Manuel Rausch[3], Ilias Bilionis[2] and Adrian Buganza Tepole[2]*

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ABSTRACT

Many natural materials exhibit highly complex, nonlinear, anisotropic, and heterogeneous mechanical properties. Recently, it has been demonstrated that data-driven strain energy functions possess the flexibility to capture the behavior of these complex materials with high accuracy while satisfying physics-based constraints. However, most of these approaches disregard the uncertainty in the estimates and the spatial heterogeneity of these materials. In this work, we leverage recent advances in generative models to address these issues. We use as building block neural ordinary equations (NODE) that -by construction- create polyconvex strain energy functions, a key property of realistic hyperelastic material models. We combine this approach with probabilistic diffusion models to generate new samples of strain energy functions. This technique allows us to sample a vector of Gaussian white noise and translate it to NODE parameters thereby representing plausible strain energy functions. We extend our approach to spatially correlated diffusion resulting in heterogeneous material properties for arbitrary geometries. We extensively test our method with synthetic and experimental data on biological tissues and run finite element simulations with various degrees of spatial heterogeneity. We believe this approach is a major step forward including uncertainty in predictive, data-driven models of hyperelasticity.

Geomechanics of the cryosphere
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ENABLING ACCELERATOR/GPU SUPPORT FOR ICE SIMULATIONS IN MPAS FRAMEWORK WITHIN ENERGY EXASCALE EARTH SYSTEM MODEL

Onkar Sahni[*1], Yuyang Gong[1], Jun Song[1], Angel Castillo-Crooke[1], Han Tran[2], Cameron Smith[1], Mark Shephard[1], Adrian Turner[3] and Deborah Sulsky[4]*

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ABSTRACT

In this presentation, we will discuss recent accelerator/GPU-enabled tools developed to perform ice-related simulations using the MPAS framework within the DOE's Energy Exascale Earth System Model (E3SM). In particular, we will present GPU-based representation and operations related to unstructured meshes, including non-uniform spherical centroidal Voronoi tessellations, and material points. We will also discuss platform portable abstraction and implementation details (for different accelerators/GPUs) that is achieved using the Kokkos library and the PUMIPic library from the SciDAC FASTMath Institute. We will focus on a C++ library, polyMPO, that we have developed to support all relevant material point/MP-related operations such as initialization of MPs, transfer of fields from mesh-to-MP and MP-to-mesh (on spherical meshes), MP tracking with specialization for a centroidal Voronoi tessellation, addition and deletion of MPs to account for freezing and melting of ice, MP migration for multi-GPU cases, etc. We will also describe our approach to interface with the MPAS code by using a well-defined set of APIs based on iso_c_binding for language interoperability between Fortran-based MPAS code and polyMPO library in C++. We will demonstrate our approach on target problems involving relevant geometries and unstructured/multi-resolution meshes on multi-GPU systems, and present performance and parallel scaling data on supercomputers.

Contact and interface mechanics: Modeling and computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

UNBIASED SEGMENT-TO-SEGMENT FRICTIONAL CONTACT ALGORITHM FOR SURFACES WITH VARIOUS DISCRETISATION TOPOLOGIES

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ABSTRACT

For the finite element-based solution of problems involving contact in physical systems, interacting bodies are commonly discretized in hexahedral or tetrahedral meshes. The decision of scheme of discretization and element topology used to do so is dependent upon the geometries of the bodies and the problem in consideration. Multiple strategies have been developed for the enforcement of contact constraints, like Node-to-Node (NTN), Node-to-Segment (NTS), and Segment-to-Segment (STS) [1]. The NTN method has limitation of being restricted in use for conformally discretized surfaces. While the widely popular NTS method [2] overcomes this limitation its use can still be disadvantageous in cases like nodes moving into blind spots, and the change of segment during sliding causing jumps in evaluated traction. While the STS method [3] overcomes these issues, it too suffers biasing with the choice of master-slave surface like NTS method, and the dual pass strategy designed to overcome this biasing can potentially lead to the inequality of the computed contact tractions. By employing a middle surface for contact traction resolution in an unbiased manner, the STS method has been utilized in this work for the solution of problems with both hexahedral and tetrahedral discretization of first and second order elements. Here, the interpenetration between contacting surfaces is penalized in the form of contact tractions which act as nodal forces on the facets of contacting elements in a manner that they maintain the force-moment equivalency and the equilibrium of contact tractions. Using regularized Mohr-Coulomb frictional law, an unbiased tangential traction calculation method is also developed for this STS method. It considers the pairs of contacting segments for any relative tangential movement and calculates the frictional forces based on elasto-plastic analogy. These implementations are tested with several benchmarks for quasi-static and dynamic cases of contact between solids in an explicit time integration framework.

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Uncertainty quantification in structural dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A SEISMIC RESPONSE PREDICTION SURROGATE MODEL WITH ENGINEERING EXPLAINABILITY USING ATTENTION-EMBEDDED CNN

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ABSTRACT

Civil structures should keep functionality during earthquake events, necessitating detailed seismic evaluations. However, to account for uncertainties in seismic loading, nonlinear time history analyses must be repeated many times, increasing the computational cost. In many studies, machine learning has been used for surrogate models to replace nonlinear time history analysis, and most of them construct surrogate models that predict only peak values. However, predicting only peak values does not capture characteristics such as frequency and energy. Therefore, some studies [1] use deep learning, often RNN, LSTM, or CNN, to predict nonlinear time history waveforms. However, deep learning has some problems, such as the black-box nature of the prediction process and the lack of attention to frequencies, which are essential from a vibration engineering viewpoint. In this study, a surrogate model is constructed from spectrograms using a CNN that incorporates an attention mechanism [2]. The spectrogram is a time-frequency feature calculated from the time history of seismic waveforms using the short-time Fourier transform. It becomes possible to understand which time-frequency features contributed to the output by using the spectrogram as input and a CNN with an attention mechanism. Specifically, an attention map is predicted from the spectrogram using a CNN, and the attention map is multiplied by the spectrogram as weights. Examining this attention map from a vibration engineering perspective improves the validity of the surrogate model. Furthermore, this study verifies the improvement in accuracy by applying convolution in the time and frequency dimensions, considering vibration engineering modeling principles. For example, features occurring later do not contribute to the response of earlier times. The verification involves constructing a surrogate model for the nonlinear response analysis under seismic loads for a lumped-mass model of a concrete pier with a seismic isolation rubber bearing and a frame model of a curved highway bridge with six-span continuous two-box girders. As results, it is confirmed that the attention map predicted from the CNN has large values around the natural frequencies, which are considered valid from a vibration engineering point of view. Vibration engineering CNN modeling is also confirmed to improve the accuracy of surrogate models.

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Boundary element methods: New theories and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BOUNDARY ELEMENT METHOD USING QUANTUM COMPUTER FOR 2D LAPLACE AND HELMHOLTZ EQUATIONS

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ABSTRACT

In recent years, there has been increasing attention on the utilization of quantum computers worldwide. However, the development of computational mechanics methods, such as the finite difference method (FDM), finite element method (FEM) and boundary element method (BEM), using quantum computers has seen little progress. Although limited, some reports have emerged on using quantum computers in the FEM [1][2][3], particularly for simple problems. It appears that utilizing quantum computers in the BEM is still rare.

Therefore, in this presentation, my recent research on the BEM using quantum computing is presented. Two types of quantum computers have been proposed: quantum annealing, developed specifically for optimization problems, and the conventional gate-based method. In this discussion, we assume that the use of the quantum gate approach. Generally speaking, it is not yet possible to execute all BEM processes on a quantum computer. Hence, we examine a hybrid computational method involving both classical and quantum computers. Currently, it seems challenging to perform pre-processing and calculate influence functions which involve the numerical integration for fundamental solutions in the BEM using quantum computers. We consider a quantum-classical hybrid computation approach where the influence function calculation is performed on a classical computer, and linear equations are encoded into a quantum computer. Linear equation Methods like the Harrow-Hassidim-Lloyd (HHL) algorithm and the Linear Combination of Unitaries (LCU) algorithm have been proposed for solving linear equations with quantum computers.

In our presentation, we will present the current state of quantum computers, some simple numerical examples using the 2-dimensional Laplace and Helmholtz equations with the HHL and LCU algorithms, and discuss future prospects and related topics.

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Physical models and reduced order models augmentation with data for physics-informed machine learning in real-world applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADAPTIVE ONLINE LEARNING WITH PHYSICS-INFORMED NEURAL NETWORKS FOR ENHANCED THERMAL PREDICTION IN METAL ADDITIVE MANUFACTURING

Pouyan Sajadi[1], Mostafa Rahmani Dehaghani[1], Yifan Tang[1] and Gary Wang[1]*

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ABSTRACT

Metal additive manufacturing (AM), a pivotal technology in modern industrial fabrication, is revolutionizing the production of metal parts through its layer-by-layer construction approach. This technique offers exceptional flexibility in design and rapid prototyping. A critical aspect of this process is the understanding and control of its thermal behavior, which significantly influences the mechanical properties and structural integrity of the final product. Accurately predicting temperature fields during the manufacturing process is thus crucial for ensuring optimal outcomes. This becomes particularly challenging with new manufacturing processes, where specific data for model training is often lacking. When we use models trained on data from previous, different processes, the results can be inaccurate. This is because these models might not fully capture the unique characteristics and variations found in the new processes.

This paper introduces a novel solution to this challenge by employing a physics-informed neural network (PINN) in an online learning framework. Our approach involves a two-phase algorithm: an initial pretraining phase and a subsequent phase of online learning. Initially, the PINN is pre-trained with datasets from known manufacturing processes with existing data, enabling the network to develop a fundamental understanding of thermal behaviors. This foundation allows the network to establish robust predictive capabilities.

Following the pretraining, the network adapts to new processes through online learning by incorporating real-time data from these processes. This adaptation is facilitated through optimization, allowing for the fine-tuning of the network's parameters in response to each unique data set. A key feature of our method is the integration of physical principles of thermodynamics into the learning process, ensuring that predictions are both data-driven and rooted in the fundamental laws of heat transfer specific to metal additive manufacturing.

This approach, which combines pretraining with adaptive online learning and a physics-informed foundation, enables our network to effectively adapt to new processes. It significantly enhances accuracy and reliability in thermal prediction, establishing a new benchmark in the application of online learning in the additive manufacturing sector. This study not only addresses the challenges of process variability but also opens doors for future advancements in theoretical adaptive control in manufacturing.

Numerical modeling of granular and multiphase flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT AND INDUSTRIAL APPLICATION OF THE ADVANCED DISCRETE ELEMENT METHOD

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ABSTRACT

The Discrete Element Method (DEM) is an innovative Lagrangian approach extensively utilized in addressing industrial challenges. Our research group has pioneered the creation of original models for the application of DEM to industrial systems. Noteworthy contributions include the introduction of the signed distance function [1] for the wall boundary model, a scaling law model exemplified by the coarse-grained DEM [2], a non-spherical particle model [3] grounded in ellipsoid principles, and the integration of an implicit algorithm to address the drag force term [4]. This presentation will showcase recent applications, such as those involving a fluidized bed [5], a twin-screw kneader [6], a three-phase fluidized bed [7], and an industrial blender [8]. Additionally, we will delve into the pivotal models pivotal for advancing the development of a digital twin for powder processes.

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Computational methods in environmental fluid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INCOMPRESSIBLE VISCOUS FLUID ANALYSIS AROUND COMPLEX SHAPES USING ISOGEOMETRIC ANALYSIS

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ABSTRACT

In Finite Element Method(FEM) analysis, low-order interpolation functions are usually used for the shape functions, which leads to shape errors in curved shapes. To address this issue, Isogeometric Analysis(IGA) [1] has recently attracted attention as an analysis method with arbitrary surfaces. IGA is effective for flow around structures with complex shapes and their fluid-structure interaction problems.

In this paper, IGA is applied to an incompressible viscous flow problem as a fundamental study. The IGA method based on multi-patches is employed; the continuity condition by superposition of Matrix Vectors is applied between patches. In order to investigate the validity and effectiveness of the present method, several benchmark problems with curves are carried out. The influence of differences in the order of the Non-Uniform Rational B-Splines(NURBS) function on numerical accuracy is investigated. The present method is also applied to the fluid-structure interaction problem. The effectiveness of IGA for viscous fluid analysis is discussed in comparison with the conventional finite element method.

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Computational mechanics for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LARGE-SCALE PHASE-FIELD SIMULATION OF CELL GROWTH IN MOLTEN POOL OF POWDER BED FUSION

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ABSTRACT

In laser powder bed fusion, the distinctive three-dimensional (3D) temperature profile in the molten pool significantly influences the morphology of dendritic/cellular microstructures. In this study, we have devised a novel model to precisely predict the 3D microstructure in the molten pool. This model bridges the meso-scale multi-physics thermal-fluid flow model [L. Wang, Y. Zhang, H. Y. Chia and W. Yan, npj Computational Materials 8 (2022) 1-11.] to the micro-scale PF model for rapid solidification of binary alloy [T. Pinomaa and N. Provatas, Acta Materialia 168 (2019) 167-177.]. To facilitate large-scale 3D PF simulations, we accelerate PF computations using the parallel computing with multiple graphics processing units (GPUs) and the adaptive mesh refinement (AMR) method (parallel-GPU AMR) [S. Sakane, T. Takaki and T. Aoki, Materials Theory 6 (2022) 1-19.]. Employing this developed model, we simulated the growth of columnar cells in the 3D thin-film cross-section domain around the bottom of the molten pool during the single-track laser scan process of an Inconel 718 plate. The simulation results were validated through comparison with experimental results and demonstrated that a characteristic 3D microstructure at the bottom of a curved molten pool can be obtained by the developed model.

AN ANALYTICAL MODEL FOR THE ANALYSIS OF DENSITY-BASED CELL-SORTING MICROFLUIFIC DEVICES IN COMBINATION WITH TRADITIONAL NUMERICAL APPROACHES

Aniol Sala[*1], Guillermo Casas[1] and Eugenio Oñate[1]*

[1]CIMNE

ABSTRACT

In this work, we present an analytic model for the analysis of density-based cell-sorting microfluidic devices. Devices of this class exploit small density variations among the various particle types to classify them. The sorting mechanism is based on maintaining a stratified flow with several fluid layers of different densities, which causes the particles to drift to their equilibrium position as they move along the circuit. Previous work relied on numerical simulations alone, as an analytical solution was not known. The model presented here predicts the density field for tubes of circular cross-section and an arbitrary number of strata with arbitrary accuracy. We discuss how it can be used to directly predict the sorting efficiency of the device in simple cases, without the need to resort to any numerical simulation. Furthermore, we consider its relevance outside its strict validity range and how it may be combined with a stabilized finite element method to produce a much more efficient hybrid method with a wider applicability range. We evaluate the accuracy of our approach against empirical data from real microfluidic devices.

16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Advances in discretization techniques, element technology, mesh adaptivity, and solution strategies for inelasticity, localization, and failure

July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN HP-ADAPTIVE PHASE-FIELD MODEL FOR FATIGUE CRACK GROWTH

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ABSTRACT

We present the numerical solution of a non-linear phase-field model for crack propagation with mesh adaptivity, discretized with the Discontinuous Petrov-Galerkin (DPG) FE methodology developed by Demkowicz and Gopalakrishnan [1].

Phase-field models have gained attention as a competitive tool to predict mesoscale morphological and micro-structure evolution in materials. In the context of crack propagation, such models provide the capability to reproduce complex crack growth patterns, such as turning, branching and merging. Unlike more traditional methods, with the phase-field approach the domain does not change as the crack grows. The use of this field parameters introduces a significant challenge: nonlinearities. The sources of nonlinearities in the selected model are two: i) The evolution of the phase-field parameter is governed by the micro-forces balance equations which are inherently nonlinear, and ii) in order to account for the discrimination of compressive and tensile stresses' contributions to the free energy, the latter must be defined by parts [2].

The DPG methodology retains various attractive features: it is a variationally flexible discretization method, that includes automatic discrete stability thanks to its optimal test functions, and has a built-in a-posteriori error estimator that naturally allows for adaptivity [3]. This results to be particularly useful for the purpose of solving phase-field models for crack growth, given the required refinements near the crack tip and near the process zone (the region of the domain where the scalar field changes from intact to damaged material zone).

While the DPG framework has been implemented for solving many models in science and engineering, only a few recent works have tackled nonlinearities. With this work, we tackle a complex problem in terms of the nonlinearities, by taking advantage of the optimal test functions.

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Mechanobiology of cells, vesicles and biomembranes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INTERACTIVE ACTIVE SURFACES: A MODEL FOR CELL AGGREGATES

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ABSTRACT

Biological tissues self-organise thanks to patterning processes coupled to cellular mechanical interactions, which play a fundamental role in driving coordinated cell movements. Here I will discuss how polarity-oriented active mechanical forces drive collective cell motion in three dimensions by modulating cell surface mechanics. I will introduce the framework of « interacting active surfaces », which describe cell aggregates as mechanically coupled flowing active surfaces. The continuum equations of active fluids, describing the flows and shape changes of the cell surfaces, are solved with finite elements. I will discuss application of this method to the three-dimensional rotational motion of cell doublets, which arise from polarised distribution of myosin motors in the cortex of the doublet cells. I will show how the interacting active surface simulation allows to capture the rotational motion of the doublet and its link with cortical flows. I will discuss how the shape of the doublet interface can be understood from an analysis of the group of symmetry of the cell doublet and application of the Curie principle. I will then discuss how principles of polarity dynamics and polarity-based mechanical interactions can act in larger three-dimensional cellular aggregates and lead to active self-assembly.

Emerging frontiers and methods in digital manufacturing: Modeling, simulation, and beyond
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATION OF DENSIFICATION-BASED FINITE ELEMENT METHOD IN CREATING DIGITAL TWIN FOR SINTERING ANALYSIS OF CERAMIC MATRIX COMPOSITES: AN INDUSTRIAL CASE STUDY

Baber Saleem[1], Ran He[1], Peter Polak[1], James Lander[2], Ian Edmonds[2], Xiaoxia Yu[1] and Jingzhe Pan[1]*

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ABSTRACT

The Densification Based Finite Element Method (DFEM) is a computational modelling technique in the field of sintering that does not rely on a full constitutive law. It utilizes densification data to predict the temporal evolution of sintering deformation in products. DFEM is advantageous when calibrating all parameters of a constitutive law is impractical for a full finite element analysis. It is not restricted to any specific sintering mechanism, making it versatile across various processes like grain boundary diffusion, vapor evaporation condensation, or liquid phase sintering. The accuracy of DFEM is comparable to that of models using full constitutive laws, making it particularly useful for proof-of-concept analyses when sintering new complex-shaped products. However, it has limitations, including its applicability only to pressureless sintering scenarios.

While DFEM has historically been applied using empirical numerical methods for calculating sintering deformation of ceramic powder compacts without detailed knowledge of viscosities and sintering potential, this research represents the first application of DFEM to an industrial part, full-scale heat shield (FSHS), using the finite element analysis. In tackling the prevalent challenge of limited data during the nascent phases of industrial development, DFEM proves to be an invaluable tool for predicting sintering distortion and shrinkage in such large-scale parts. This expansion of DFEM's application, showcased on a Rolls-Royce demonstrator part, marks a significant advancement in its practical utility. In conjunction with the DFEM digital twin of FSHS, the study proposes sintering boundary conditions to suppress real-time distortion.

Large-scale structural and fluidic topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HARNESSING ADVANCED CFD AND ML COMPILER TOOLS FOR TOPOLOGY OPTIMIZATION OF LARGE-SCALE FLUID THERMAL PROCESSES

Hesam Salehipour[1], Massimiliano Meneghin[1], Mohammadmehdi Ataei[1], Pradeep Kumar Jayaraman[1], Nigel Morris[1] and Adrian Butscher[1]*

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ABSTRACT

Topology optimization (TO) of real engineering flows requires robust CFD algorithms that are highly optimized for maximum performance and include advanced capabilities to handle high Reynolds number flows, wall models, complex boundary conditions, and coupled physics for fluid-thermal processes. The adjoint computations, which are an essential part of gradient-based topology optimization, must be equally efficient and equipped with the same advanced capabilities to be useful for realistic design optimization purposes.

In many ways, the computational challenges of TO algorithms are similar in principle to those faced by the AI community where large-scale models need to run efficiently in both forward and backward modes to perform gradient descent optimization.

In this talk, we will present how recent compiler technologies developed for ML research (such as JAX and Pallas frameworks) may be leveraged to produce a massively parallelizable adjoint CFD solver based on the Lattice Boltzmann method (LBM). Our proposed solution, namely XLB [1, 2], leverages the solver's differentiability and is highly extensible in Python. We will demonstrate results of level-set-based topology optimization for a wide range of problems that incorporate advanced LBM techniques and capture coupled fluid-thermal physics with arbitrarily complex objectives and constraints. The efficient multi-GPU performance of forward and backward computations, that are key for large-scale TO problems, will also be highlighted.

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Uncertainty quantification and scientific machine learning for predictive modeling of complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DIGITAL TWINNING IN COMPUTATIONAL CARDIOLOGY

Matteo Salvador[*1], Fanwei Kong[1], Mathias Peirlinck[2] and Alison Marsden[1]*

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ABSTRACT

In recent years, blending physics-based modeling with data-driven methods has had a major impact on digital healthcare. Several frameworks have been proposed to create certified digital replicas of different areas of the cardiovascular system. These computational pipelines include multiscale and multiphysics mathematical models based on differential equations, machine learning methods to build accurate and efficient surrogate models of cardiovascular function, sensitivity analysis, and parameter inference with uncertainty quantification. Here, we show the potential of Branched Latent Neural Maps (BLNMs), a recently proposed scientific machine learning tool, to learn complex space-time fields coming from physics-based models, and how these simple and compact feedforward partially connected neural networks can be effectively deployed for personalized medicine. BLNMs have different advantages. Indeed, they use additional latent outputs to improve the learned space-time dynamics, they break the curse of dimensionality, and they retain excellent in-distribution generalization over an arbitrary discretization. Several applications of BLNMs for digital twinning in computational cardiology will be shown.

Machine learning for large scale models in physics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NONLINEAR REDUCED BASIS APPROXIMATION OF DISCRETE CONTACT PROBLEMS IN CROWD MOTION

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ABSTRACT

In this work we develop new model reduction approaches to predict the solutions of time-dependent parametrized problems describing crowd motion in the presence of obstacles.

The problem of interest is described by a discrete contact model (DCM), which is formulated as a constrained least-squares optimization statement: the particles velocity field is seeked as the projection of the spontaneous velocities of each particle into a feasibility set (which prevents the overlap between particles and between particles and obstacles).

The parametric variations in the problem are associated with the geometric configuration of the system and to the initial positions of the particles: they have a dramatic impact in the solution, both in terms of positions and contact forces. We investigate new developments of the reduced-basis method and supervised machine-learning techniques to effectively find, in a decorrelated manner, primal and dual reduced spaces: to do so, we rely on a non-linear reconstruction from the first coordinates of a linear reduced basis approximation.

To assess the validity of the method, the nonlinear compressive strategy is then compared to more standard linear and nonlinear approximations.

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Advanced discretization schemes and solution strategies for computational structural dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A SPACE-TIME FINITE ELEMENT FORMULATION FOR LARGE DISPLACEMENT PROBLEMS WITH COMPUTATIONAL COSTS EQUIVALENT TO TIME-MARCHING METHODS

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ABSTRACT

This study introduces a space-time finite element formulation for solid mechanics, featuring specially designed quadratic shape functions in the time direction. The approach employs the time-slab concept, where trial functions within each slab are determined by nodal parameters of velocity and position at the initial time-slab boundary and position at the final time-slab boundary. Each time-slab is independently solved, taking velocity and position values from the preceding slab final boundary as initial conditions, with the position nodal values at the current time-slab's final boundary as unknowns. As a result, the number of unknowns is the same as in standard time marching methods with identical spatial finite element discretization. Three different options are explored for selecting test functions with the same shape functions of positions, while restraining distinct test function nodal parameters. These choices result in diverse stability and dissipation characteristics. To evaluate the numerical characteristics of the method, we firstly perform testing with linear 1D problems, and following, we apply it to develop a space-time finite element formulation for 2D elasticity with large displacements, using a total Lagrangian description and taking the current nodal positions as main variables. The proposed approach has computational cost similar to the standard time-marching approaches, demonstrating favorable convergence rates and stability. Future applications are anticipated for more intricate nonlinear problems.

key-words: space-time finite element method, large displacements, Lagrangian description

Finite element techniques for wave simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SYMPLECTIC HAMILTONIAN HYBRIDIZABLE DISCONTINUOUS GALERKIN METHODS FOR LINEARIZED SHALLOWS-WATER EQUATIONS

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ABSTRACT

We propose a new hybridizable discontinuous Galerkin method for approximating the linearized shallow-water equations. The discretization aims to preserve relevant physical quantities such as mass, vorticity, and energy. Specifically, we reformulate the system of equations in a Hamiltonian form, employing Hybridizable Discontinuous Galerkin Methods (HDG) for spatial discretization and obtaining a semi-discrete scheme written in Hamiltonian form. By leveraging on the inherent Hamiltonian structure of the numerical method and implementing symplectic time-marching schemes, we ensure the conservation properties of the fully discrete system of equations. We discuss the fundamental properties of our analysis and present numerical experiments to validate its performance.

Geomechanics of the cryosphere
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GRAPHICS PROCESSING UNIT ACCELERATED ICE FLOW SOLVER FOR UNSTRUCTURED MESHES USING THE SHALLOW SHELF APPROXIMATION (FASTICEFLO V1.0.1)

Anjali Sandip[1], Ludovic Räss[2] and Mathieu Morlighem[3]*

[1]*University of North Dakota*
[2]*University of Lausanne*
[3]*Dartmouth College*

ABSTRACT

Ice-sheet flow models capable of accurately projecting their future mass balance constitute tools to improve flood risk assessment and assist sea-level rise mitigation associated with enhanced ice discharge. Some processes that need to be captured, such as grounding line migration, require high spatial resolution under the kilometer scale. Conventional ice flow models mainly execute on central processing units (CPUs), which feature limited parallel processing capabilities and peak memory bandwidth. This may hinder model scalability and result in long run times requiring significant computational resources. As an alternative, graphics processing units (GPUs) are ideally suited for high spatial resolution as the calculations can be performed concurrently by thousands of threads, processing most of the computational domain simultaneously. In this study, we combine a GPU-based approach with the pseudo-transient (PT) method, an accelerated iterative and matrix-free solution strategy, and investigate its performance for finite elements and unstructured meshes with application to two-dimensional (2-D) models of real glaciers at a regional scale. For both Jakobshavn and Pine Island glacier models, the number of nonlinear PT iterations required to converge a given number of vertices N scales in the order of N1.2 or better. We further compare the performance of the PT CUDA C implementation with a standard finite-element CPU-based implementation using the price-to-performance metric. The price of a single Tesla V100 GPU is 1.5 times that of two Intel Xeon Gold 6140 CPUs. We expect a minimum speed-up of at least 1.5x to justify the Tesla V100 GPU price to performance. Our developments result in a GPU-based implementation that achieves this goal with a speed-up beyond 1.5x. This study represents a first step toward leveraging GPU processing power, enabling more accurate polar ice discharge predictions. The insights gained will benefit efforts to diminish spatial resolution constraints at higher computing performance. The higher computing performance will allow running ensembles of ice-sheet flow simulations at the continental scale and higher resolution, a previously challenging task. The advances will further enable quantification of model sensitivity to changes in upcoming climate forcings. These findings will significantly benefit process-oriented sea-level-projection studies over the coming decades.

Advances in neural operators for scientific modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A UNIFYING FRAMEWORK FOR OPERATOR LEARNING VIA NEURAL FIELDS

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ABSTRACT

Operator learning is an emerging area of machine learning which aims to learn mappings between infinite dimensional function spaces and has led to the development of new architectures such as the Fourier Neural Operator, the DeepONet, and their extensions. In this work we uncover a previously unrecognized connection between existing operator learning architectures and conditioned neural fields used in computer vision. This results in a unified framework for explaining differences between popular operator learning architectures, and creates a bridge for adapting well-developed tools from computer vision for operator learning. In particular, we find all existing operator learning architectures are neural fields whose conditioning mechanisms are restricted to use only pointwise and/or global information. This motivates us to design new architectures which make use of a hierarchy of scales for conditioning a base neural field. By making use of multi-scale conditioning, we observe consistent performance gains and obtain state of the art results across a collection of challenging benchmarks in climate modelling and fluid dynamics.

Model order reduction for parametrized continuum mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ON METAHEURISTIC STRUCTURAL OPTIMIZATION WITH PARAMETRIC MODEL ORDER REDUCTION

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ABSTRACT

Design optimization involving complex structures can be a very resource intensive task. The present work focuses on the non-convex optimization problem involving eigenvalues that arises in structural design optimization. Parametric Model Order Reduction (PMOR) was identified as a potential tool for improving the efficiency of the optimization process. For the buckling eigenvalue problem, we turned to meta-heuristic approaches due to the non-linear dependence of the geometric stiffness matrix on the design variables. A two-step optimization procedure was developed. In the first, a set of projection vectors that can be used to project the solutions of the governing higher order partial differential equations to a lower manifold is assembled. Invariant components of the system matrices that do not depend on the design variables were identified and reduced using the projection vectors. In the second (online) step, particle swarm optimization (PSO) was carried out. Here, the buckling analysis problem for each design is assembled and solved directly in the reduced form. Applicability of this approach to the design of variable angle tow fiber composite structures was investigated and an efficient matrix decomposition for the linear stiffness matrices was derived to aid in this process. PMOR-based optimization exhibited a 0.55% relative error compared to full order model-based studies and similar convergence history. The optimization efficiency was improved by 64.41% with a reduction of 86.57% in eigenvalue analysis time and 99.8% in memory requirements, affirming PMOR's suitability for global optimization of VAT fiber composite structures. Further improvement in computational time is expected with current work on deriving an affine decomposition for geometric stiffness matrix. Investigations are also being carried out on the impact of PMOR on the convergence properties of PSO.

Computational methods in environmental fluid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MULTIDIMENSIONAL MODELING FRAMEWORK FOR ASSESSING COMPOUND INUNDATION THROUGH A REDUCED-PHYSICS APPROACH IN COASTAL WATERSHEDS

Felix Santiago-Collazo[*1], Logan Bayer[1] and Matthew Bilskie[1]*

[1]*University of Georgia*

ABSTRACT

Water is vital for any civilization to prosper; thus, settlements have been established within the coastal or fluvial floodplain throughout history. These communities, especially low-gradient ones, are prone to flood hazards such as nuisance flooding, storm surges, extreme rainfall, and high river discharge. However, compound inundation occurs when two or more flood drivers (e.g., coastal and hydrological) coincide or are in close succession. Consequently, the flood impacts during these events can be exacerbated due to the nonlinear interaction of the coastal and hydrologic processes. However, current numerical modeling approaches are not suited to capture this intricate relationship accurately by coupling different models for each process.

This research presents a unified approach for compound flood assessments based on a reduced-physics numerical scheme. This unstructured finite element model simulates coastal, fluvial, and pluvial processes that employ the full or a reduced form of shallow water equations. As a first step, a one-dimensional (1-D) approach was employed in idealized coastal watersheds to understand better the physical processes and their interaction during a compound flood event. This reduced-physics modeling approach employs the kinematic wave equations (KWE) to simulate overland runoff in the watershed and riverine flow in non-estuarine locations. In contrast, the diffusive wave equations (DWE) are applied to simulate riverine flow in estuarine regions to account for backwater processes. Lastly, the complete shallow water equations are applied in the coastal areas for simulating astronomical tides and storm surges. Next, the lessons learned from the 1-D approach were extended to a two-dimensional (2-D) approach by developing a hydrologic model based on the reduced-physics approach. This model uses a finite element spatial discretization (e.g., symmetrical weak weighted residual) and a Crank-Nicolson scheme for time discretization.

Initial results highlight the nonlinearity of the flood processes within a compound flood event. This nonlinearity may be attributed mainly to the peak levels occurring at different times for each flood driver. However, the time-to-peak water levels of all the individual flood scenarios arrive within an hour at the exact location, but the linear superposition overestimates the total inundation. Therefore, the non-linearity depends not only on the time-to-peak water levels but also on the momentum exchange. By improving this relationship between flood drivers in a compounding flood event, holistic modeling frameworks can be developed and serve as a critical planning tool for decision-makers, stakeholders, and authorities.

Advances in material model calibration for computational solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CALIBRATION OF A RATE-DEPENDENT CONCRETE MATERIAL MODEL USING HIGH-VELOCITY IMPACT EXPERIMENTS AND SURROGATE-BASED OPTIMIZATION

Jean Santiago-Padilla[*1], William Lawrimore*[1], Jesse Sherburn*[1] *and Andreas Frank*[1]

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ABSTRACT

The U.S. Army's ERDC has developed an advanced concrete material model adept at capturing multiple rate-dependency effects, as well as complex damage mechanisms encompassing macro- and micro-cracking. This allows for better prediction of concrete behavior under extreme loadings such as blast and projectile impact, which is of great interest to the U.S. Army in the design of their protective structures. However, one of the challenges with this new material model is the inability to constrain certain strain-rate parameters through standard lab tests. A solution is to leverage carefully designed high-velocity impact experiments to calibrate these unconstrained material model parameters. In this work, an inverse method using surrogate-based optimization is proposed to calibrate ERDC’s concrete model to a series of terminal ballistic experiments with rigid ogive penetrators. To do this, numerical simulations using the EPIC hydrocode are run through an optimization workflow in the Dakota framework. The design parameters are the material model coefficients, while the objective is to minimize error between simulated acceleration-time histories and experiments. Computational analysis includes a factor screening to determine each parameter’s effect on the response metric, a parametric study testing different surrogate models and optimization algorithms, and an assessment of design feasibility when adding physical constraints on the concrete’s strain energy. To check robustness, the resulting calibrated model is then validated against an additional set of experiments with impact conditions not considered in the optimization process.

Modeling and simulation of dynamics, stability and control of aerospace structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MINIMIZATION OF VIBRATIONS IN AERONAUTICAL WING SPARS UNDER FLUTTER SITUATION

Larissa Santos[1], Marcelo Araujo Silva[1] and Reyolando Brasil[1]*

[1]*Federal University of ABC*

ABSTRACT

The present work aims to study the mitigation of vibrations of aeronautical wing spars in cases of flutter. For these cases will be studied aero elasticity, which is defined as the science that is interested in the mutual interaction between elastic, aerodynamic and inertial forces in a body on aerodynamic flow. Among aeroelastic phenomena, flutter can be defined as the self-excited interaction between two or more modes of vibration of a properly altered system. This is fed back by the flow of a fluid, which can, at certain speeds (flutter speed), result in a tragic failure. This occurs due to the development of oscillations of increasing amplitudes, impairing the performance and safety of the aircraft, which can lead to a failure of the structure. This is a critical problem faced by aircraft designers, especially in the design of those structures where high performance is required. In this case, it is necessary to reduce the weight and control the aerodynamic loads. Thus, an analytical method was developed through the equation of motion for a typical section with two degrees of freedom: torsion and flexion. The flutter velocity for the studied aircraft problem was obtained through the analysis of the stiffness and mass matrices, obtaining a V-f diagram in addition to the damping values as a function of the velocity V. Finally, a degree of freedom was added to the system, corresponding to a TMD (Tunned Mass Damper), which aimed to increase the flutter speed using optimization techniques. With this, the aircraft could have a greater range of speeds for Operation. Suggestions for future work were also proposed.

Advanced analysis of steel and steel-concrete composite structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HUMAN COMFORT ASSESSMENT OF PEDESTRIAN FOOTBRIDGES BASED ON THE USE OF DESIGN RESPONSE SPECTRA

Paula Oliveira Bezerra Diniz[1], Jorge Maurício Souza[1], Amanda Borges Oliveira[1], Gilvan Lunz Debona[2] and José Guilherme Santos da Silva[1]*

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ABSTRACT

The pedestrian footbridges are more and more becoming the modern landmarks of urban areas. The designers seem to continuously move the safety border, aiming to increase the pedestrian footbridges slenderness and lightness. However, more and more footbridges are carried out as light weight structures with low frequencies and low damping. These facts have generated very slender footbridges, sensitive to dynamic excitations, and consequently changed the serviceability limit states associated to the design. In general, the current design codes and guides recommend the use of deterministic models to assess the dynamic behaviour of footbridges. On the other hand, the effect of the uncertainties in mass, stiffness and damping of the investigated structure are relevant and lead to uncertainties on the values of the footbridges natural frequencies. Nevertheless, the human walking is a stochastic phenomenon and the dynamic force generated at each step depends of the weight, the step frequency and the step length of each pedestrian. This way, this research work aims to contribute with the structural designers based on the development of a probabilistic approach to assess the dynamic behaviour of footbridges considering the stochastic nature of the pedestrian's walking, in order to evaluating the structural response with regard to excessive vibrations that may cause human discomfort. Based on the use of probabilistic methods, it becomes possible to determine the probability of the footbridge's peak acceleration values exceeding or not the human comfort criteria. The results obtained in this investigation reveal that the values of maximum accelerations calculated based on the deterministic methods may be overestimated in design situations.

New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

3D STRUCTURAL FOUNDATION DESIGN FOR ONSHORE WIND TURBINES VIA TOPOLOGY OPTIMIZATION

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ABSTRACT

Structural foundations for onshore wind turbines face the dual challenge of balancing structural integrity with cost efficiency. While opting for a robust foundation with substantial mass to ensure a stiffer structure may be tempting, this approach often translates to higher costs. In this context, this work proposes a topology optimization methodology for 3D designs of onshore wind turbine foundations. The primary objective is to design optimized structural foundations considering a maximum concrete volume constraint. The analysis encompasses considerations for both static and dynamic loads. The structural foundation is designed over a large portion of soil beneath the wind turbine, designated as the design domain. Material properties within the design domain are defined based on binary decision variables, denoted as {1} for concrete or {0} for soil. The soil-structure problem is solved through the Finite Element Method, employing the Perfectly Matched Layer (PML) approach to absorb dynamic waves and simulate an infinite domain. Different volume fractions of concrete are explored. The sensitivities of the problem are calculated using semi-automatic differentiation, and the Topology Optimization of Binary Structures with Geometry Trimming (TOBS-GT) method is employed to solve the {0,1} optimization problem via Integer Linear Programming. The numerical results show the effectiveness of the proposed methodology in designing cost-effective 3D structural foundations and its potential to provide useful insights into onshore wind turbine foundations.

Current trends in phase-field modeling and computations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHASE-FIELD MODELING OF FATIGUE BASED ON MICROMECHANICS APPROACH

Mina Sarem[1], Nuhamin E. Deresse[1], Jacinto Ulloa[2], Els Verstrynge[1] and Stijn Francois[1]*

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ABSTRACT

This presentation addresses the development of a micromechanics-base phase-field model for characterizing fatigue failure in (quasi-)brittle materials, as fatigue stands as an important cause of fracture in engineering structures. The phase-field variational method is utilized to simulate and regularize the complex, discontinuous functions governing the physics of cracks. Despite its computational benefits, the phase-field approach has limitations, such as the inability to distinguish between tensile and compressive failure, potentially leading to the development of unrealistic crack patterns in compression. In this study, we employ a framework that enhances the phase-field model by integrating a micromechanics-based approach [1, 2]. This combination helps to differentiate between failure modes without adopting heuristic modifications, by distinguishing between open and closed microcracks. This framework links macroscale field variables, such as plastic strain and damage variable, to micromechanical mechanisms like frictional sliding and opening of microcracks.
Our primary focus is to incorporate accumulation of fatigue damage and deterioration caused by cyclic loading into the micromechanics-based phase-field model. To achieve this, we first improve the algorithm's stability for loading-unloading in the tensile regime by modifying the plasticity evolution equations. Additionally, we introduce a fatigue degradation function to the model, which degrades the fracture energy upon reaching a specified threshold during cyclic loading [3]. Various cyclic loads are applied to benchmark tests to capture diverse failure modes. Our results demonstrate the model's capability to accurately simulate the main features of fatigue behavior, including crack nucleation, growth, and coalescence.

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REVISITING THE ISSUE OF ENERGY CONSERVATION IN PHASE-FIELD MODELS FOR FRACTURE

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ABSTRACT

Phase-field models for fracture have become very popular in recent years due to their innate ability to predict the path of crack propagation and their robustness with regard to topological challenges associated with crack nucleation, branching and coalescence. However, enforcing energy conservation in the event of brutal cracking remains an open problem. Even in problems involving purely quasi-static loading, it is well known that the resulting fracture evolution may nevertheless include both stable and unstable crack growth. In the latter case, a naive solution of the governing equations in the corresponding simulations leads to a loss in the total potential energy: an apparent violation of the energy conservation law. This energetic signature is not limited to crack nucleation events, but can also be observed in connection with the finite (as opposed to infinitesimal) extension of an existing crack. Previous attempts at recovering energy conservation involved the use of backtracking schemes based on a global energy minimization principle, however such schemes can lead to unphysical results including violation of Griffith's criterion.

In this talk, we present an alternative paradigm aimed at recovering energy conservation without resorting to global minimization. Instead, we take into account the fact that unstable crack growth is an inherently dynamic phenomenon, and adopt a heuristic approach to include such dynamic effects within an otherwise quasi-static framework. This enables us to avoid having to solve the full dynamic linear momentum equation, and additionally also allows us to simulate crack evolution anywhere within the spectrum defined by full energy conservation at one end, and maximal energy loss at the other. We compare numerical results obtained using the proposed framework to recently published experiments, as well as results obtained with classical phase-field approaches.

Recent advances in computational fracture mechanics and failure analysis
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A STATE-OF-THE-ART REVIEW ON THE RECENT ADVANCES OF AN EFFECTIVE FINITE ELEMENT TOOL FOR FRACTURE ANALYSIS

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ABSTRACT

The computation of fracture mechanics parameters has always been challenging for the people working in this field. Besides the ongoing improvements demonstrated by commercial software, many research groups have dedicated themselves to developing their in-house codes. A particular example of such codes was given in the past by introducing FRAC3D program to the fracture community [1]. As a specialized finite element software, FRAC3D benefits from enriched elements to determine fracture parameters. The advantage of this program over other similar software is the accuracy levels obtained by using much less elements around the crack region. Hence, the main objective for the users of this program has been to increase its capabilities for covering a wide range of fracture-related problems. Recently, several developments for this program were demonstrated by using various fracture examples. The dynamic version of the program was used to simulate the stress wave propagation phenomenon and compute time-dependent fracture parameters for straight and curved crack fronts. On the other hand, a parallel version of the same code was created by using multiprocessing (MPI) tools and this was shown with the aid of the fracture analysis of an electronic packaging structure [2]. Another interesting problem involves the computation of welding residual stresses on a specific component with external welding software, and then the determination of residual stress effects on fracture parameters for the same geometry with a stationary crack that is subjected to a subsequent load [3]. The latter part of that study was realized by using FRAC3D with necessary implementations. Current investigations concentrate on the details for the incorporation of residual stress effects and crack growth simulations. Having an efficient tool for this purpose seems very significant considering the complexities associated with this type of analysis.

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SCALABLE MIXTURE MODEL APPROXIMATIONS FOR NONLINEAR SPARSE BAYESIAN LEARNING

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ABSTRACT

The nonlinear sparse Bayesian learning (NSBL) algorithm permits the automatic discovery of optimal nested models [1]. Inspired by applications in engineering for nonlinear-in-parameter models, NSBL generalizes the concept of relevance vector machines permitting the inclusion of informative priors for a priori relevant parameters while leveraging the use of Gaussian automatic relevance determination (ARD) priors for parameters of questionable relevance. The optimal model is thus revealed by pruning irrelevant parameters. This is achieved by optimizing the parameters of the ARD priors (the hyperparameters). The efficiency of the algorithm relied on the use of a Gaussian mixture model (GMM) approximation for the product of the likelihood and informative priors which permits the derivation of semi-analytical expressions for several Bayesian entities for nonlinear models, with non-Gaussian priors or likelihood functions. Expressions for the parameter posterior pdf, the model evidence, and the NSBL objective function can be derived in terms of the GMM kernel parameters and the hyperparameters.

The success of the NSBL algorithm critically depends on the construction of the GMM approximation. Kernel density estimation or clustering methods can be used to construct a GMM using Markov Chain Monte Carlo samples. While this can accurately capture non-Gaussian attributes and correlation between parameters, these methods are computationally expensive and do not scale well. Conversely, variational methods adopting mean-field approximations scale well, but generally discards critical information on the correlation structure of the posterior which is critical for sparse learning. Towards developing scalable implementations of NSBL, we consider the use of the global optimization and Laplace approximation (GOLA) algorithm [2] for the construction of the GMM. This methodology was recently proposed as a warm-start for variational inference. Here we investigate the suitability of this approach for the purpose of constructing the NSBL objective function as necessary component of the optimal model discovery.

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Phase-field modeling: Analytics, benchmarks, and discussions
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL MODELLING OF STEAM GENERATOR ROLLED PLUG USING PHASE FIELD APPROACH

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ABSTRACT

Rolled plugs are elements used for defected steam generator tubes plugging to prevent leakage of radioactive water from the primary circuit into the environment by forming leak tight seal with the tube. They are installed inside the tube using rolling process which causes plastic deformation of the plug shell made out of Inconel 690 TT. Hot temperature, high pressure, flow-induced vibrations, primary water stress corrosion cracking and transient conditions during startup and shutdown of nuclear power plant affect rolled plug structural integrity and can have impact on the plug performance. Additionally, the impact of the irradiation-hardening must be taken into consideration. 60-year lifespan of the rolled plug which must meet requirements of the new generation of nuclear power plants adds to the significance of the material fatigue and degradation mechanisms which affect component lifespan. The critical area of the plug represents deformed rolling area in contact with the tube where material fatigue is expected to exhibit.

Common approaches for material fatigue are based on stress-life, strain-life and linear elastic fracture mechanics principles. Recently, phase field method has become immensely popular for modelling of material fatigue and fatigue crack growth prediction, based on the energy release rate [1]. At the same time, it can accurately capture material fatigue while taking into consideration thermo-mechanical material properties [2].

The conducted research will provide more information about the impact of the rolling process on the plug fatigue, which can also be used for steam generator tube rolling process simulations and research. Phase field method will provide more detailed insight into harsh nuclear power plant primary circuit conditions which act on the rolled plug performance during whole 60-year lifespan and the safety of the components inside the primary circuit of the nuclear power plant.

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Computational methods in environmental fluid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING HURRICANE STORM SURGES USING RADIAL BASIS FUNCTIONS: A MESHLESS APPROACH

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ABSTRACT

Accurately predicting storm surges holds paramount importance for coastal communities grappling with rising sea levels and more frequent extreme weather events. Traditional numerical methods such as Finite Difference, Finite Element, and Finite Volume methods are widely employed for these simulations but face challenges in generating meshes, particularly when handling complex coastlines with rapidly changing bathymetry. In contrast, meshless methods have emerged as a viable alternative, gaining traction in recent years due to their ability to bypass the intricate and laborious steps of mesh generation.

This abstract presents a meshless approach utilizing the radial basis function (RBF) method to solve the shallow water equations (SWEs) and simulate storm surges. The method offers flexibility in node placement and eliminates numerical issues related to element/cell quality. Our method employs a method-of-lines formulation, wherein surface derivatives inherent to the SWEs are locally approximated using RBF interpolation. Additionally, we utilize polyharmonic splines as a radial basis function to circumvent the requirement of specifying an arbitrary shape parameter. This presentation will delve into the intricacies of the RBF method, highlighting its unique capabilities. We will discuss several test cases to showcase the effectiveness and efficiency of our proposed approach in accurately predicting storm surges.

Immersed-boundary variational methods: Theory, data structures, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ON REMESHING AND DATA TRANSFER IN THE FINITE CELL METHOD

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ABSTRACT

The numerical analysis of complex geometries in finite element analysis can be challenging because the generation of boundary-conforming meshes of good quality is important to obtain reliable results. This meshing process can be simplified by using immersed-boundary methods such as the finite cell method (FCM). In the FCM the domain is discretised with a Cartesian mesh using high order shape functions. The discontinuity introduced by the immersed boundary requires special treatment during numerical integration. In addition, cells with a low volume fraction tend to distort severely during the numerical analysis. This can be particularly problematic for finite strain analysis, where the tangent stiffness matrix is computed in the deformed state. The large distortions can then cause convergence problems for the incremental/iterative solver.

One way to heal the distorted cells is to apply remeshing. This will be discussed in this presentation, including an analysis of different methods for data transfer during the remeshing process.

Quantum scientific computing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

QUANTUM ALGORITHM FOR TIME-EVOLVING PARTIAL DIFFERENTIAL EQUATION VIA HAMILTONIAN SIMULATION

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ABSTRACT

Partial Differential Equations (PDEs) serve in modeling the dynamic behavior of various physical phenomena such as solid mechanics, heat conduction, and fluid dynamics. In contemporary engineering, solving these equations as fast as possible for extremely large-scale systems is crucial for advancing industrial developments. Despite the evolution of supercomputers, solving PDEs for extensive systems within a reasonable timeframe remains a formidable challenge.

Quantum computing, an area garnering significant interest over recent decades, is recognized for its potential to execute computations much faster than classical computers. Although current quantum computers face limitations in hardware scalability and noise resistance, significant advancements in hardware performance have been observed. Notably, quantum computing shows great promise as an efficient solver for PDEs.

In steady-state, PDEs reduce to systems of linear or non-linear equations solvable by linear system solvers. Among the quantum algorithms applicable to these problems, two types are predominantly considered: variational quantum algorithms and the so-called Harrow-Hassidim-Lloyd (HHL) algorithm [1]. Variational quantum algorithms are tailored for near-term quantum devices and have undergone extensive research for PDE applications. Conversely, HHL-based algorithms require fault-tolerant quantum computers, offering theoretical advantages over classical algorithms under specific conditions. For time evolution problems, near-term and long term-quantum algorithms have also been proposed. Variational quantum simulation is a representative method for near-term devices while Hamiltonian simulation is a counterpart for long-term ones [2].

Given the recent progress of hardware toward the era of early fault-tolerant quantum computers, we focus on Hamiltonian simulation for partial differential equations. Specifically, we propose an algorithm for explicitly constructing quantum circuits of time evolution operators for Hamiltonian described by spatial difference operators. The key concept of our method is to quantize PDEs into the qubit system and perform time evolution on the Bell basis. In our presentation, we will showcase several numerical experiments to demonstrate the validity and effectiveness of our proposed method. These experiments suggest the capability of quantum algorithms to handle large-scale PDEs efficiently, which we believe not only advances the field of quantum computing but also opens new avenues in computational mechanics.

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Computational modeling of cardiac fibrosis: A multiscale, multiphysics challenge
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NETWORK DYNAMICS OF CARDIAC INFLAMMATION-FIBROSIS COUPLING

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ABSTRACT

Inflammation and fibrosis are conserved phases of wound healing in the heart, skin, and other organs. Yet therapeutic attempts at manipulating inflammation and fibrosis have had limited success, indicating a need for greater understanding of how inflammation and fibrosis are controlled by intracellular and intercellular molecular networks. In this talk, I will present our computational and experimental systems biology research on cardiac inflammation and fibrosis. These studies include large-scale computational models of the intracellular signaling networks in fibroblasts, macrophages, and most recently neutrophils, as well as simulations of their intercellular interactions that predict how cardiac cells coordinate inflammation-fibrosis coupling. These computational models highlight a critical role of fibroblast proliferation and its regulation by the scavenger receptor LRP1 via Src and JNK signaling. Our computational models are validated with experimental data from the literature as well as new experiments with fibroblast proliferation and a new fibroblast-specific LRP1 deletion mouse model after myocardial infarction.

Computational fluid dynamics (CFD) and fluid-structure interaction (CFSI): Methods and Applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A CURVILINEAR SURFACE ALE FORMULATION FOR NAVIER-STOKES FLOW ON DEFORMING SURFACES

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ABSTRACT

A new arbitrary Lagrangian-Eulerian (ALE) framework for fluid membranes, such as soap films, bubbles and lipid bilayers, is presented. These membranes are characterized by in-plane fluid flow and out-of-plane elasticity. This leads to the challenging task of describing fluid flow, such as incompressible Navier-Stokes flow, on evolving surfaces. The new formulation extends the surface ALE formulation of [1] to more general surface motions. It is based on a new curvilinear surface parameterization that describes the motion of the ALE frame. Its in-plane part becomes fully arbitrary, while its out-of-plane part follows the material motion of the surface. This allows for the description of flows on deforming surfaces using only surface meshes. The unknown fields are the fluid pressure, fluid velocity and surface motion, where the latter two share the same normal velocity. The new theory is implemented in the nonlinear finite element framework of [2] using the stabilization scheme of [3] for the incompressibility constraint. The implementation is verified through several manufactured steady and transient solutions, obtaining optimal convergence rates in all cases.

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Advances in damage & fracture modeling of multiphysics materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CHEMO-MECHANICAL MODEL FOR STRESS CORROSION CRACKING ACCOUNTING MICROSTRUCTURAL HETEROGENEITY

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ABSTRACT

Stress corrosion cracking (SCC) is one of the most unforeseen phenomena that can result in the catastrophic breakdown of load bearing components in harsh environments across multiple engineering sectors. This occurs primarily because of arbitrary progression of corrosion pits leading to fracture and thus, the ultimate load carrying capacity of structural members for its service life is significantly compromised. Therefore, enlargement of the pits and associated SCC is a strongly coupled chemo-mechanical phenomena. Notably, the development of the complex SCC profile is observed to be substantially influenced by intrinsic microstructural characteristics, such as grain boundary character, grain size and crystallographic texture. Although numerous experimental and numerical studies have been performed to investigate the intertwined SCC phenomena, the influence of microstructural features on the corrosion evolution and subsequent formation of fracture is not addressed rigorously. Therefore, it is utmost necessary to unlock SCC with respect to material heterogeneity and external environmental and mechanical loading conditions towards the service life assessment of the mechanical component.

In the present work, a thermodynamically consistent chemo-mechanical model is developed to account for the evolution of corrosion, deformation and crack formation in heterogeneous materials. The classical Allen-Cahn equation is considered adopting a phase field descriptor for the corrosion field while the phase field fracture method is applied for crack propagation. In the phase field method, the sharp interface is modeled through a continuous field variable. The non-equilibrium thermodynamics will be employed to extract the constitutive relationships and driving forces for evolution laws of order parameters describing corrosion and fracture of material. Using variational principle, the weak forms of the coupled governing equations are extracted. Employing finite element procedure, the discretized equations are obtained for displacement, phase field order parameter for corrosion and phase field variable for fracture. Utilizing Newton-Raphson based staggered iterative procedure, the linearized set of coupled equations will be developed and solved efficiently through an in-house developed parallel computing simulation platform. Upon generating various polycrystalline microstructures, the corrosion pit growth and its transition into crack will be simulated. The effect of crystal orientation will be accounted for in corrosion kinetic parameters as well as elastic moduli. A systematic parametric study will be performed to investigate spatial evolution of the stress corrosion cracking for various grain sizes in different electrochemical conditions under applied external deformation. Finally, predictive estimation of remaining service life will be accomplished for load bearing elements with various chemical and mechanical conditions.

Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HOW DO STRUCTURE AND MATERIAL AFFECT MECHANICAL STRENGTH OF ADDITIVELY MANUFACTURED BONE SCAFFOLDS?

Venus Savaliya[*1], Zhongpu (Leo) Zhang[1], Chunhui (Richard) Yang[1], Kejun Dong[1] and Qing Li[2]*

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ABSTRACT

The emergence of Additively manufactured, commonly referred as 3D printed, bone scaffolds provides a novel treatment avenue for the patients experiencing severe bone infections or injuries from accidents in absence of autografts or allografts as viable options. The effectiveness of these scaffolds hinges on their ability to mimic the natural bone extracellular matrix environment and promote bone regeneration. Kalsi, Singh & Kumar Sehgal emphasize the importance of achieving structural, physiological, chemical, and mechanical similarity to genuine bone for an optimal scaffold [1]. This study is dedicated to assessing the mechanical strength of four alternative scaffold structures and their compatibility with the additive manufacturing (AM) process.

In this study, 20 × 20 × 20 mm3 scaffolds, with diverse structural designs and a porosity of 65%^±0.5, are designed using Dassault Systèmes SolidWorks software. Hexagon Simufact Additive software will be employed to simulate the AM process, capturing deformation and residual stresses in the scaffold structures for both 17-4PH and ceramic materials. Subsequently, numerical models from Simufact will be transferred to Simulia ABAQUS for mechanical testing to assess the mechanical strength of the scaffold structures. The results for each structure and material will be compared to discern their behaviour under loading conditions and their compatibility with AM.
The study aims to evaluate the impact of the AM process on mechanical strength compared to conventional manufacturing techniques and investigate the influence of scaffold structure and material on overall mechanical strength.

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Machine learning methods for multiscale and multiphysics material modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MICROSTRUCTURE-INFORMED DATA-DRIVEN MODELING OF MECHANICAL BEHAVIOR OF COLD-SPRAYED ADDITIVELY MANUFACTURED METAL-CERAMIC COMPOSITES

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ABSTRACT

This study aims to develop a microstructure-based data-driven model to predict the stress-state and- strain-rate-dependent mechanical response of Al-Al2O3 composites fabricated by cold spray additive manufacturing (CSAM). Multiscale finite element modeling is leveraged to generate rich datasets for the training/validation process of the data-driven model. Accordingly, representative volume elements (RVEs) informed by the microstructural characteristics (e.g., Al2O3 particle weight fraction, Al2O3 particle size distribution, and porosity in the Al matrix) of the CSAM composite are randomly generated. For the Al matrix and Al2O3 particle, constitutive material models were implemented by a VUMAT subroutine in Abaqus/Explicit finite element (FE) solver that accounts for the effect of stress state and strain rates on the material failure behavior. The micromechanical FE model was validated with experimental data regarding stress-strain curves and observed failure mechanisms under quasi-static and dynamic loading. Once validated, the multiscale framework was exercised across the space of design variables (i.e., microstructural features) and loading conditions (i.e., stress states and strain rates) for generating datasets for the training and validation of an artificial neural network (ANN); this ANN model correspondingly correlates the macroscale mechanical response of the composite material to its microstructural characteristics. The outcomes indicated that the developed multiscale data-driven model successfully reconstructs the stress-state- and strain-rate-dependent stress-strain response of the material as a function of microstructure. Overall, the current microstructure-based data-driven model has profound implications for the computationally efficient design and optimization of CSAM metal-ceramic composites for clean technology and aerospace applications through (1) Bridging the scales by paving the way for the establishment of a micromechanism-based ML-enabled constitutive model that is implementable in commercial FE packages as a user-subroutine applicable to structural scale modeling, and (2) Being leveraged as a surrogate model in conjunction with multi-objective genetic optimization algorithms for the computationally-assisted design of the material with tailored mechanical properties.

EVALUATION OF CARDIAC FIBROSIS AND INTERVENTION USING COMPUTATIONAL BIOMECHANICS

John Sayut[1], Javiera Jilberto[1], Mia Bonini[1], Will Zhang[1] and David Nordsletten[1]*

[1]*University of Michigan*

ABSTRACT

Chronic heart failure is often caused by irreparable damage to the myocardium, leading to a progressive decline in cardiac function and patient outcomes. Given the global shortage of donor hearts, researchers look to engineered solutions including fabricated tissue patches, stem cell seeding, and devices [1]. The fabrication of heart muscle remains a challenge - with cardiomyocyte maturation and formation of tissue structure loosely approximating adult heart muscle [2]. However, it remains unclear how much benefit could be derived from current engineered muscles in vivo and how to prioritize optimization of structure and function.

Bridging between engineering and application, computational biomechanics enables quantification of the relative influence of maturation and structure on whole organ function. To understand this relative influence, we developed a model by coupling a biventricular solid mechanical model to a zero-dimensional Windkessel systemic flow model [2]. The material law selected represents cardiac tissue properties of viscoelasticity, compressibility, and muscle contraction. To model fibrosis and intervention, a simulated transmural fibrotic patch is defined in the basolateral region of the left ventricle with a linearized border zone. Finite element simulations investigate the driving factors behind functional improvement with alterations to contractility, patch material parameters, and patch fiber orientation.

Each model is studied throughout the cardiac cycle, including an analysis of cardiac functional indicators such as ejection fraction and stroke work. Results show that contractility is a principal contributor to cardiac function - improved myocyte response to activation signals can impressively recover over half of ejection fraction with a purely circumferential myofiber orientation. In addition, the data does also indicate that native fiber alignment improves cardiac function. The native transmural variation better matches the native biomechanics, driving the twisting behavior characteristic of cardiac contraction. Additionally, native hyperelastic stiffness improves cardiac function, especially in the diastolic filling phase. This information illustrates the key engineering decisions facing the current state of cardiac tissue engineering and fibrosis treatment.

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Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPLETE VARIABLE KINEMATIC CUF-BASED MULTILAYERED SHELL ELEMENTS

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ABSTRACT

Shells structures play a crucial role in various engineering applications owing to their efficient load-bearing capacities. However, the evolution of structural materials, such as composite materials, has led to more intricate designs, necessitating rigorous analyses, which lead to a considerable rise in computational costs.

The complexity of analysing these structures primarily arises from anisotropic nature, leading to intricate mechanical phenomena. These problems include challenges such as ensuring continuity between layers for shear components and meeting zig-zag distribution requirements for displacements, commonly known as C0z requirements [1]. The combination of out-of-plane and in-plane strain components increases the intricacy. Thus, the classical theories cannot accurately study such structures. Scholars proposed several refined theories for composite structures, employing two primary modelling techniques: the Equivalent-Single Layer (ESL) and the Layer Wise (LW) approaches. In the ESL approach, mathematical assumptions regarding the displacement field remain consistent across all layers. Consequently, the resulting model encompasses variables for the entire composite structure. Conversely, the LW approach involves distinct variables described in each layer, while ensuring mechanical characteristics' continuity at the interlaminar level.

The primary objective of this study is to approach shell analysis from a new perspective, wherein each displacement field can be approximated using an appropriate structural theory. For instance, employing advanced LW theories for in-plane displacements and ESL models for transverse displacements. The Carrera Unified Formulation (CUF) [2] serves as the tool enabling the implementation of each theory in a simple and hierarchical manner within a Finite Element (FE) framework The novel CUF uses nine scalar Fundamental Nuclei, whose formulation does not change with the chosen kinematic theory.

The study comprehensively analyses shells, ranging from thick to thin structures. To counteract the shear and membrane locking of the FE methods, the Mixed Interpolation of Tensorial Components is implemented in the formulation [2]. The analysis employs nine-node Lagrangian elements as shape functions and considers diverse boundary conditions and loading types. Both displacement and stresses can be accurately described. The results lead to interesting conclusions: (a) it is possible to reduce computational costs using only the significant terms; (b) the number of effective variables depends on the specific problem; (c) implementing the Mixed ESL/LW approach proves to be efficient.

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Computational methods in environmental fluid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STORM SURGE MODELING ON THE FJORDS OF NORWAY WITH ADCIRC

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ABSTRACT

Storm surge and coastal hazards can have devastating consequences for a coastal nation like Norway, especially considering sea level rise due to climate change. Since 2011, the Norwegian Directorate of Civil Protection (DSB) has been publishing guidelines on dealing with these issues in local planning.[1] We present a finite element model, which is necessary to better understand and predict the impacts of storm-induced flooding in Norway.

The Norwegian Meteorological Institute (MET) has been modeling the coast for a variety of applications; however, both of these models are difficult to scale to higher resolutions. The finest one, NorKyst-800, has a resolution of 800 meters, and while they both model the shallow-water equations, they use a uniform grid with finite difference methods.[2] The global finite element model, STOFS-2D, is still relatively coarse in Norway.[3]

In order to better model the complexity of Norway's fjords, a much finer coastal resolution is required. We can then see the effects of flooding further into the fjords, and eventually allow for more complex models, such as compound flooding. To this aim, present a new grid of Norway's coast at a variety of resolutions, down to about 30 meters, including limited topography information to assist with flood modeling.

We use the Advanced CIRCulation model (ADCIRC) with these new meshes to simulate the effects of tides and winds along the shoreline, beginning with a smaller-scale mesh of the Oslo fjord, and continuing with the full coastal mesh. The results from these are compared to the results from NorKyst-800, as well as MET water level gauges in various locations.

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Multiphysics and data-driven modeling for cardiovascular biomedicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN FSI SIMULATION OF VENTRICLE AND AORTA INTEGRATING IN-VIVO AND IN-SILICO DATA

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ABSTRACT

The development of digital twins of the cardiovascular (CV) system presents several challenges, for example, in achieving custimization to induvidual patients. While Fluid-structure interaction (FSI) models represent one of the best high-fidelity tools for this purpose, their practical application is often constrained by the necessity of multiple patient-specific parameters that remain unknown. Although medical imaging provides large amounts of in-vivo data, its full integration into in-silico models still faces several problems.

This study employs data assimilation techniques to merge dynamic CT scan data with an FSI simulation to create a high-fidelity digital twin of a patient's left ventricle (LV) and aorta. An ECG-gated CT scan of a patient is used to obtain segmentations of the aorta and LV lumen boundaries at each of the 20 cardiac phases acquired. Lagrangian markers are defined on these surfaces and tracked over time employing a gradient-based registration method [1]. Data-driven FSI simulations are performed using an in-house code based on the Immersed Boundary method [2]. Data assimilation is applied to the dynamics of the CV structures to conform to in-vivo kinematics. A variation of the Nudging technique [3] is developed to simultaneously integrate local and integral measurements. For anatomical regions where in vivo data is accurate, local measurements guide each Lagrangian marker. Conversely, in areas with less reliable data, nudging is applied to follow integral measurements, such as tracking the LV volume over time.

The methods used in this study allow for the accurate reproduction of the kinematics of the cardiovascular structures, which is crucial in capturing hemodynamics as well. The method effectively transitions from a purely FSI-based simulation to one driven by kinematics, offering enhanced adaptability in the simulation process. This flexibility allows for testing various scenarios to derive the most precise outcomes.

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Computational and analytical advances in nonlocal modeling
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NOVEL QUADRATURES IN CONTINUUM-KINEMATICS-INSPIRED PERIDYNAMICS

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ABSTRACT

Continuum-kinematics-inspired peridynamics (CPD) [1] is an extension to peridynamics (PD) [2] that can capture the Poisson effect correctly and in addition does not suffer from zero energy modes. (C)PD is a nonlocal continuum mechanics formulation, where every continuum point interacts with continuum points in its finite-sized neighbourhood, the so-called horizon. CPD, in contrast to PD, classifies the interactions in one-, two- and three-neighbour interactions dependent on the number of contributing neighbours. Considering the change in pair-length, triplet-area and tetrad-volume allows CPD to be a geometrically exact formulation and to reflect the Poisson effect in 2D and 3D problems.

The nonlocal interactions between continuum points result in integro-differential governing equations that depend consequently on the integration over the horizon. It is difficult to solve the integro-differential equations analytically, which is why numerical methods need to be exploited. In (C)PD models, the continuum is typically discretized by a finite number of so-called collocation points, at which the governing equations are evaluated. The collocation points can additionally serve as integration points for the quadrature of the horizon. This method is commonly used for (C)PD models despite its dependence of the integration accuracy and computational cost on the discretization. To address this problem, we established a novel quadrature for (C)PD, where the integration and collocation points no longer necessarily coincide. To do so, we align the integration points in a hexagonal pattern for 2D problems and evaluate the governing quantities at the integration points by interpolating the governing quantities of the collocation points with either linear or quadratic interpolation schemes. Thus, our novel quadrature of the horizon in 2D has a fixed number of six integration points and is independent of the discretization of the continuum with respect to the computational cost.

We validate the accuracy of our novel quadrature by various numerical examples. The results of the novel quadrature show a good accuracy and are in good accordance with the results obtained with the quadrature dependent on the discretization, while the computational cost is reduced tremendously. In future work, we want to extend our approach to 3D problems.

3D-ACA FOR THE TIME DOMAIN BOUNDARY ELEMENT METHOD: COMPARISON OF FMM AND H-MATRIX BASED APPROACHES

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ABSTRACT

The time domain boundary element method (BEM) for the homogeneous wave equation with vanishing initial conditions is considered. The generalized convolution quadrature method (gCQ) developed by Lopez-Fernandez and Sauter [2] is used for the temporal discretisation. The spatial discretisation is done classically using low order shape functions. A collocation approach is applied for the Dirichlet problem and a Galerkin approach for the Neumann problem.

Essentially, the gCQ requires to establish boundary element matrices of the corresponding elliptic problem in Laplace domain at several complex frequencies. Consequently, an array of system matrices is obtained. This array of system matrices can be interpreted as a three-dimensional array of data which should be approximated by a data-sparse representation. The multivariate Adaptive Cross Approximation (3D-ACA) [1] can be applied to get a data sparse representation of these three-dimensional data arrays. Adaptively, the rank of the three-dimensional data array is increased until a prescribed accuracy is obtained. On a pure algebraic level it is decided whether a low-rank approximation of the three-dimensional data array is close enough to the original matrix. Within the data slices corresponding to the BEM calculations at each frequency either the standard H-matrices approach with ACA or a fast multipole (FMM) approach can be used. The third dimension of the data array represents the complex frequencies. Hence, the algorithm makes not only a data sparse approximation in the two spatial dimensions but detects adaptively how much frequencies are necessary for which matrix block.

In the presentation, this methodology is recalled and both versions either using H-matrices in the slices or FMM will be compared. The study is numerically performed at selected examples as the mathematical analysis gives the same complexity. Nevertheless, the performance of the algorithm differs.

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ADVANCING DATA-INTEGRATED TIME STEP ESTIMATION TO IMPROVE SIMULATION PERFORMANCE

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ABSTRACT

In explicit finite element simulations for structural dynamics, a stable computation is only possible when the chosen time step is smaller than the critical time step of the discretized system. However, computing the critical time step exactly by solving the corresponding eigenvalue problem is numerically too expensive. To circumvent this, there are several approaches to estimate the critical time step of a system, many of them through an estimation on the element level.

One widely used inexpensive approach is the estimation of the critical time step of a finite element via heuristic formulas based on geometric quantities. By means of these a characteristic length is calculated for an element. An estimate for the critical time step is then obtained by dividing this characteristic length by the wave speed.

For instance, the characteristic length of a 2D solid element can be calculated by the element area divided by its longest side or its longest diagonal. However, the resulting time step estimate is not necessarily conservative, which necessitates the introduction of a safety factor to prevent simulation instabilities. For more complex elements the estimate can be even less accurate, as many influencing factors may be neglected when heuristic formulas are used.

On the contrary, data-integrated time step estimation [1, 2] utilizes representative data sets of all relevant element shapes to develop new, accurate time step estimators. Building upon the concept of data-integrated time step estimation, this contribution extends the methodology to a broader range of finite elements and situations, showcasing the adaptability and reliability of the method. Our goal is to demonstrate the effectiveness of data-integrated time step estimation to find accurate time step estimators for complex finite elements. Through our work, we show how this approach can enhance simulation speed and simulation robustness in real-world engineering scenarios.

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Advances and applications in meshfree, particle, and peridynamic methods
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A COUPLED LAGRANGIAN/SEMI-LAGRANGIAN QUASI-CONFORMING EMBEDDED RKPM WITH SMOOTH CONTACT ALGORITHM FOR MODELLING PENETRATION PROBLEMS

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ABSTRACT

Key Words: Reproducing Kernel Particle Method, Meshfree Methods, Lagrangian Embedded Methods, Immersed Methods, Quasi-Conforming, Smooth Contact, Energy-Based Contact Algorithm, Multi-Body Contact

We present a coupled Lagrangian/semi-Lagrangian (L-SL) [1], quasi-conforming embedded reproducing kernel particle method (QCE-RKPM) [2] with an enhanced RK smooth contact algorithm [3] for modelling penetration problems. Due to the extreme deformation caused by the penetration process in the form of fracture, fragmentation, and localized shear, the semi-Lagrangian RKPM is utilized only in the areas of extreme deformation, while a Lagrangian RKPM description is used elsewhere. This coupling maintains accuracy in the approximation while improving computational efficiency. Furthermore, the quasi-conforming embedded technique is employed which combines adaptive refinement in the penetrated material ahead of the projectile's path with a variational consistency correction that allows two non-conforming discretizations in contact to pass the contact patch-test thus improving the accuracy and convergence of the contact algorithm. Lastly, RK smooth contact, a node-to-surface contact algorithm which constructs a smooth master surface using the RK approximation for greater accuracy and stability in the contact force and master surface approximation, is enhanced by utilizing spherical representations of the slave nodes and employing an energy-based contact formulation for enforcing the impenetration constraints. This enhancement improves contact detection for coarse slave discretizations while reducing the effect of mesh-dependency. These coupled techniques offer a robust and efficient computational framework for modelling penetration problems.

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Immersed-boundary variational methods: Theory, data structures, and applications
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ERROR-CONTROLLED MULTI-LEVEL HP FINITE CELLS IN THE REALM OF ELASTOPLASTIC ANALYSIS

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ABSTRACT

The idea of hp-refinements has established as the method of choice for the analysis of non-smooth solution fields in the finite cell method [1] to ensure a stable and reliable convergence behavior in both, linear and non-linear analysis. In the context of higher order approximation, an adapting hp-refinement over multiple overlay meshes has proven to be an extremely valuable extension, overcoming many of the issues from the established refinement techniques [3, 2].

In this talk, we present an extension of the adaptive multi-level hp-refinement to plasticity problems. Moreover, we show an efficient error-control method to decide about the cell-wise need for refinement [2]. The presented approach allows for an independent local h- and p-refinement to improve the solution in smooth and non-smooth regions of the problem domain. The local refinements are performed automatically through different error- estimators based cell-specific measures. We assess the performance of the proposed method with benchmark problems and compare our results to other established refinement approaches. Finally, we demonstrate the applicability of our extensions with problems from the engineering routine.

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SIMULTANEOUS EQUATION OF STATE PARAMETER CALIBRATION AND ESTIMATION OF EPISTEMIC UNCERTAINTIES IN EXPERIMENTAL DATA

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ABSTRACT

This study aims to simultaneously calibrate the parameter values, with uncertainty, in the Davis Reactants Equation of State (EOS) and estimate epistemic uncertainties in experimental data for the high explosive (HE) PBX 9501.

Bayesian methods are often used to calibrate EOS parameters with uncertainty given experimental data [1-2]. However, it is not uncommon for those experimental data to have poorly characterized uncertainties or be provided without uncertainty information altogether. A common solution is to assume 10% error on the experimental measurements, but this is just a guideline and might not be applicable for any given dataset. Thus, we seek to estimate the experimental errors from the data within the calibration problem.

In this study we formulate the Bayesian parameter calibration as a constrained optimization problem where we seek the EOS parameter values and experimental errors which maximize the log-posterior probability. The types of experimental data used to form the likelihood for the calibration include Hugoniot, specific heat capacity, and thermal expansion tests on the HE and its components. The constrained optimization problem was solved with Sequential Least Squares Programming.

We found optimal posterior EOS parameter values that are consistent with previously calibrated values for the same material [3] and improve the fit of the EOS to the experimental data compared to the prior. We also estimated that the experimental errors range between 5% - 30% depending on the dataset, so the 10% error assumption is not appropriate for all the considered datasets. This study provides a framework for simultaneously calibrating model parameters and estimating epistemic uncertainty in the form of unknown experimental errors.

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Applications of shape optimization in complex engineering problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTI-MATERIAL TOPOLOGY OPTIMIZATION WITH CONFORMAL ANALYSIS MESHES

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ABSTRACT

The promise of Topology Optimization (TO) is to provide engineers with a systematic computational tool to support the development of optimal designs. Multi-material topology optimization further allows for a larger design space and as such may result in better performing designs. Moreover, multi-material optimization enables the efficient design of active structures. A shortcoming of classic density based multi-material TO designs is the nebulous interphase region between materials, which leads to inaccurate response predictions in these very regions. In contrast, designs based on boundary and interface regions, rather than interphase regions, yield accurate response predictions.

In this study, we develop a multi-material Level-set (LS) topology optimization approach in which geometries are described through the iso-contour of one or multiple LS fields which are discretized over a mesh. The nodal heights, serve as the design parameters. The governing field equations are discretized by a conformal discretization over a separate “analysis” mesh. In the optimization, the “analysis” mesh is morphed such that its boundary and interfaces conform with the isocontours of the LS fields. The mesh morphing is performed using the Target-Matrix Optimization Paradigm (TMOP) approach. Our TMOP formulation is a PDE based mesh morphing operation which aims to improve the interface conformity while preserving mesh quality. Design sensitivities of the optimization cost and constraint functions with respect to all design LS fields are computed through an adjoint approach which accounts for the mesh morphing process. Higher-order basis functions are used for discretizing both the governing equations and the LS fields. The proposed analysis and optimization framework is based on MFEM, a free, lightweight, scalable C++ library for finite element methods which supports the optimization of large-scale optimization problems.

We investigate the robustness of the proposed optimization methodology by solving two- and three-dimensional multi-material optimization problems involving linear diffusion and elasticity. We discuss the advantages and challenges of our approach with regards to the mesh morphing process. Finally, select aspects and challenges of our approach with respect to parallel computing and processor decomposition are discussed.

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CONFIGURATIONAL FORCES FOR EFFICIENT CRACK GROWTH SIMULATIONS WITH THE VIRTUAL ELEMENT METHOD

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ABSTRACT

The virtual element method (VEM) [1] is an efficient discretization scheme for the numerical solution of boundary value problems on polytopal grids, which is most prominently known for offering considerable flexibility in the discretization process. In the context of numerical applications of fracture mechanics, one of its most attractive features results from the possibility to employ elements of complex shape with an arbitrary number of nodes, which may be convex as well as non-convex and may even contain crack tips. Consequently, crack growth simulations with the VEM benefit from the fact that incremental changes in the geometry of a crack do not require any remeshing of the structure, but rather crack paths can run through already existing elements, enabling the realization of very efficient simulations in terms of computational cost.
Although the method provides a valuable tool for modelling crack propagation, there is still research required regarding the implementation of efficient and precise methods to evaluate crack tip loading quantities and crack deflection criteria. Therefore, the concept of configurational forces in material space is employed, which already proved to be very efficient for the calculation of these quantities in the context of the FEM. However, the calculations yield certain numerical difficulties that need to be dealt with, e.g., due to discontinuous stresses and strains at element edges in the vicinity of the crack tip, and require additional effort in connection with curved crack faces [2].
This work aims to discuss theoretical and computational aspects of employing configurational forces for mixed-mode crack growth simulations in the VEM. A framework for calculating nodal configurational forces is presented and comparative studies are conducted, carefully investigating challenges and opportunities emerging from the discretization method for assessing crack tip loading and crack path prediction. Furthermore, virtual elements are modified to align their approximation power with the singular behaviour at crack tips in linear elastic fracture mechanics. Crack growth simulations are presented, and results are compared to reference solutions as well as solutions obtained with the FEM.

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Phase-field modeling: Analytics, benchmarks, and discussions
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BENCHMARK STUDY ON CHEMO-ELASTIC MULTIPHASE-FIELD APPROACHES

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ABSTRACT

A number of challenges and issues arises when modeling multicomponent and multiphase solid alloy systems. Multiphase-field methods provide a numerically efficient framework for the prediction of microstructure evolution without the need for grain boundary tracking. Due to their usage in a wide range of fields and their constant development it is crucial to establish standardized benchmarks. Within this work, a series of chemo-elastic equilibrium stages for Fe-C binary alloys is discussed. These simulations contribute to the development of standard benchmarks that validate separately as well as the combination of chemical, capillary, and mechanical driving forces. To this end, a multiphase-field model with chemo-elastic coupling is employed [3]. Sharp interface solutions are recovered by mechanical driving forces employing the jump condition approach [2] and chemical driving forces based on the grand potential density [1]. The Gibbs free energy is approximated using parabolic functions that incorporate parameters from a Calphad database. Thermodynamic and mechanical equilibrium conditions are provided by the sharp interface formulation. The Gibbs-Thomson equation provides an interfacial equilibrium condition. Analytical solutions are derived from these conditions and compared with phase-field simulations.

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PHASE-FIELD MODELLING OF FATIGUE FRACTURE CONSIDERING INHOMOGENEOUS MATERIAL PROPERTIES

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ABSTRACT

We present a comprehensive investigation into the phase-field simulation of fracture accounting for inhomogeneous material properties. Fracture mechanics plays a pivotal role in understanding the structural integrity of materials, and the phase-field approach provides a powerful framework for capturing crack propagation in a continuous and numerically efficient manner. However, incorporating realistic variations in material properties poses a significant challenge for accurately predicting fracture behavior in heterogeneous structures.

Our study addresses this challenge by integrating a phase-field fracture model with a detailed representation of inhomogeneous material properties. Therefore, we consider the example of Tooth Flank Fracture in case hardened spur gears (TFF) [1]. We adopt a phase-field model that combines classical fatigue damage calculation with the phase-field method [2,3], allowing for the simulation of fatigue crack initiation and propagation in materials with spatially varying mechanical properties. The proposed methodology accounts for the impact of material heterogeneity on crack initiation location, fracture patterns, critical load cycle numbers, and crack paths. The numerical framework is validated against experimental data, demonstrating its capability to capture complex fracture phenomena in the strongly inhomogeneous example of TFF. A more detailed investigation requires the consideration of the actual microstructure to understand crack initiation and early crack growth more. We therefore showcase the versatility of our approach by a general study on the incorporation of resolved microstructures. In a first step the choice of numerical solvers, modelling strategy and general challenges of the extension of phase-field fracture simulations to lower material scales are discussed. Relevant numerical examples are shown and underline the necessarily statistical evaluation of such simulations.

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Modeling friction and wear
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MATERIAL REMOVAL OF A CONVEX PATTERN SURFACE INTERACTING WITH NON-SPHERICAL PARTICLES: A NUMERICAL STUDY

Yunpeng Yan[12], Skirmantas Pargalgauskas[1], Rudy Helmons[1] and Dingena Schott[1]*

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ABSTRACT

A convex pattern surface is proposed and optimized to mitigate the sliding wear of bulk handling equipment caused by interaction with bulk solids. This work investigates the effectiveness of the convex pattern surface on wear reduction during interactions with non-spherical particles. Multiple representative particles, obtained through a sampling method, are reconstructed using a photogrammetry technique. Two contact parameters between particles are calibrated through shear box and drawdown tests to ensure flow behavior similar to the real material. The numerical results indicate that the convex pattern surface can effectively reduce wear compared to a plain sample when involving both spherical and non-spherical particles. For a plain sample, the wear volume remains independent of particle shapes and increases linearly with numerical revolutions. For the convex pattern surface, the wear volume demonstrates a quadratic relationship with the test revolutions as the deformation of convex elements weakens the effectiveness of the sample on wear reduction. The particle flow behavior analysis reveals that the convex pattern surface experiences the lowest wear volume when in contact with non-spherical particles. This can be attributed to the non-spherical particles sliding shorter distances and rotating with higher angular velocities on the convex pattern surface.

Advanced materials and smart structures: Modeling, simulation and testing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING OF DAMAGE IN FIBER-REINFORCED HIGH-PERFORMANCE CONCRETE AT LOW CYCLE FATIGUE USING A PHASE-FIELD REGULARIZATION

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ABSTRACT

Fiber-reinforced high-performance concrete (HPC) shows a pseudo-ductile material be- havior during failure, mainly characterized by complex fiber-matrix interactions. We propose a phenomenological material model to discuss the influence of reinforced fibers, represented by orientation distribution functions (ODF), on the failure process of HPC. Therein, an additive type macroscopic energy function is formulated, superimposing the models of one-dimensional elastoplasticity for the steel fibers and an elastoplastic phase- field fracture model, cf. [1], which can predict the nonlinear behavior of high-performance concrete (HPC) during low-cycle fatigue. We apply the pressure-sensitive Drucker-Prager yield criterion as a basis for pure concrete behavior. A phase field model is used to reg- ularize the softening behavior of the material; otherwise, we can expect a pathological response in the finite element method. Two different data-driven degradation functions are calibrated to model the asymmetric tension-compression behavior of HPC, see [2]. Three-point bending experimental tests at low-cycle using notched beams are performed, and the experimental load-CMOD (crack mouth opening displacement) curves are used to calibrate the proposed numerical model. ODFs approximate different distributions and orientations of reinforced fibers, see [3]. The accuracy of the proposed numerical model is verified by comparing the degradation of stiffness in numerical and experimental results.

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Advanced discretization schemes and solution strategies for computational structural dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MATRIX-FREE HIGHER-ORDER FINITE ELEMENT SOLVERS IN TISSUE MECHANICS

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ABSTRACT

Finite element methods play a fundamental role in science and engineering, where low-order approximations are particularly prominent for practical applications. Classical algorithms rely on matrix-based iterative solvers and related preconditioners for implicit solution. However, the time-to-solution of such implementations is mainly determined by memory bandwidth, which determines the speed at which the precomputed and stored matrix entries can be loaded from main memory to evaluate sparse matrix-vector products within iterative solvers. Since modern computer architectures can execute more than 100 arithmetic operations for each variable transferred from memory, so-called matrix-free approaches are getting increasingly attractive. These methods redundantly evaluate the action of the linear operator from the underlying finite element integrals on a vector (see, e.g., [1, 2] for general nonlinear solvers for nodal high-order finite elements). First, such schemes were developed for fluid-mechanics problems building on results of the spectral element community, but recent advances [3, 4] have shown that they can also be fruitfully applied to solid mechanics problems.

Within this work, we focus on static nearly-incompressible hyperelasticity considering anisotropic effects stemming from dispersed fibers as often applied in the context of tissue mechanics. Starting from [3], which focused on isotropic compressible hyperelasticity, we extend the concept towards the nearly-incompressible anisotropic case. A matrix-free approach is presented, combining sum-factorization and tensor-product continuous, higher-order finite elements with hp-multigrid preconditioned Krylov methods. A purely displacement-based approach is chosen, weakly enforcing incompressibility via a penalty term.

The classical total Lagrangian form and an alternative reformulation based on integration in the spatial configuration are investigated in terms of their computational efficiency. These alternative formulations constituting the linearized operator are carefully evaluated in terms of relevant performance metrics, comparing to a matrix-based implementation with an algebraic multigrid preconditioner. We show that matrix-free methods for finite-strain hyperelasticity are indeed promising in both benchmark problems from biomechanics and patient-specific models of vascular tissue, while user adaptations of the constitutive law can be accomplished being largely agnostic toward the remaining implementation.

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Simulations of particle-laden fluid flows
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A HIGH-ORDER EULER-LAGRANGE APPROACH FOR PARTICLE-LADEN FLOW IN MOVING DOMAINS

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ABSTRACT

Compressible flows with suspended particles occur in a wide variety of applications, e.g., spray injections or aeronautical engineering. Many of these applications can include rotating geometries and/or the altering of component's surfaces through, e.g., icing or erosion, resulting in complex, highly transient multiscale and multiphysics problems. One of the challenges of such problems is to adequately describe the time-resolved coupling between the chosen moving mesh approach and the particle method, while maintaining the efficiency of the resulting numerical scheme.
In this talk, we present the extension of our high-order accurate massively parallel discontinuous Galerkin spectral element framework FLEXI [1,2] towards particle-laden flows in moving domains. The framework is based on the Euler--Lagrange approach and has been previously applied to wall-resolved large-eddy simulation of high-Reynolds number flows with a one- and two-way coupled dispersed particulate phase, delivering accurate results while maintaining excellent scaling up to tens of thousands cores. Rotating geometries will be represented by a sliding mesh method, while for the altering of component's surfaces, a mesh movement based on the arbitrary Lagrangian-Eulerian approach is chosen. Special care is taken to retain the optimal scaling properties of FLEXI. This work concludes by presenting examples of large scale computations for particle-laden flows in complex, possibly moving systems and giving an outlook on the next research challenges.

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Advanced computational modelling of wood, wood-based products, bio-composites, and timber structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FINITE ELEMENT METHOD AND FRACTURE MECHANICS-BASED SIMULATION OF BRITTLE FAILURE MODES OF CONNECTIONS IN TIMBER STRUCTURES

Caroline D. Aquino[1], Michael Schweigler[2], Leonardo G. Rodrigues[3], Jorge M. Branco[1] and Thomas K. Bader[2]*

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ABSTRACT

For the design of robust timber buildings, it is essential to develop reliable methods to assess possible brittle failure of connections. Therefore, in this contribution a three-step modeling approach was implemented in the ABAQUS finite element software to predict (i) the single fastener behavior, (ii) the stress distribution between fasteners and (iii) brittle failure of the timber in laterally loaded connections with steel dowels and slotted-in steel plates. The local nonlinear behavior of single-dowel connections was determined utilizing a beam-on-foundation (BoF) approach [1]. In the subsequent step, the timber member and the steel plate were modeled using 3D shell elements with linear-elastic orthotropic and isotropic material properties, respectively. In this step, the load-displacement behavior of the single-dowels from the BoF model was represented by nonlinear springs located at the connection shear planes. The interaction between rigid cylinders, representing the dowel, and the 3D shell elements, representing the timber and steel members, was characterized by defining hard contact in the normal direction and friction in the tangential direction. To evaluate potential brittle failure of the timber, a post-processing module was integrated into a Python script based on the mean stress method utilizing linear fracture mechanics as proposed by Gustafsson [2]. The stress distribution was obtained for each load increment during the numerical analysis. Subsequently, the mean stress length was calculated for various potential failure paths along the grain direction. The failure criteria were assessed for each pre-defined path and load increment to identify the critical path and estimate the connection's load-bearing capacity. The numerical model accurately fitted previous experimental tests regarding load-carrying capacity and connection slip. The novel combination of modeling the nonlinear connection behavior with the finite element method and assessment of potential brittle failure with linear fracture mechanics, gives access to a realistic load distribution among the fasteners in a multiple-fastener connection, for a reliable prediction of crack initiation in the timber matrix, while taking advantage of high computational efficiency.

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Modern structure-preserving methods for PDEs
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NEURAL GALERKIN SCHEMES THAT CAN PRESERVE HAMILTONIANS AND OTHER QUANTITIES

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ABSTRACT

Neural Galerkin schemes, based on the Dirac-Frenkel variational principle, train nonlinear parametrizations sequentially in time to approximate solution fields of time-dependent partial differential equations. Due to the nonlinearity of the parametrizations, few parameters efficiently capture even complex dynamics in first-principles-based physical models. Such models are often constructed based on the observation that quantities like energy, mass, and momentum remain constant over time, representing conserved quantities of the physical system. In this talk, we demonstrate how we can modify Neural Galerkin schemes such that these quantities are also conserved quantities in the approximate solutions produced by Neural Galerkin schemes.

We first show that only adding constraints that aim to conserve quantities in continuous time can be insufficient because the nonlinear dependence on the parameters implies that even quantities that are linear in the solution fields become nonlinear in the parameters and are thus not conserved by standard Runge-Kutta time integration schemes. Instead, we propose Neural Galerkin schemes that compute an embedding onto the manifold of nonlinearly parametrized solution fields that conserve given quantities at each time step. We present numerical experiments that show the effectiveness of our proposed method to preserve given quantities up to machine precision. The talk is based on our preprint [1].

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Computational and analytical advances in nonlocal modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NONLOCAL BOUNDARY VALUE PROBLEMS WITH LOCAL BOUNDARY CONDITIONS

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ABSTRACT

We state and analyze nonlocal problems with classically-defined, local boundary conditions. The model takes its horizon parameter to be spatially dependent, vanishing near the boundary of the domain. We establish a Green's identity for the nonlocal operator that recovers the classical boundary integral, which permits the use of variational techniques. We show the existence of solutions, as well as their variational convergence to classical counterparts as the horizon uniformly converges to zero. In certain circumstances, global regularity of solutions can be established, resulting in improved modes and rates of variational convergence. We also show that Galerkin discretization schemes for the nonlocal problems converge unconditionally with respect to the nonlocal parameter, i.e. that the schemes are asymptotically compatible.

Isogeometric methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A SHIFTED BOUNDARY APPROACH TO ISOGEOMETRIC ANALYSIS ON TRIMMED SURFACES

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ABSTRACT

Isogeometric Analysis (IGA) has established itself as a very successful framework for computational mechanics, with broad applications to fundamental and industrial problems. In recent years, great focus has been dedicated to the application of IGA to CAD models which include trimmed surfaces. One of the challenges that trimmed surfaces pose is that they make the geometric description with NURBS more complex. It is for this reason that immersogeometric techniques have been pursued, which however require the integration of the IGA variational forms on cut NURBS supports. We present an alternative approach based on the recently developed Shifted Boundary Method. Complex data structures and integration on cut elements are avoided by means of an approximate boundary representation and a modification (shifting) of the boundary conditions via Taylor expansions. This approach maintains optimal accuracy while greatly simplifying the practical implementation. We show a prototypical example in the context of the Poisson equation.

Emerging frontiers and methods in digital manufacturing: Modeling, simulation, and beyond
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BEYOND LUBRICATION FLOW FOR THIN-FILM MANUFACTURING

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ABSTRACT

Reynolds' hydrodynamic lubrication theory has been used extensively to analyze and quantify thin-film manufacturing (Roberts et al. 2013). Applications span liquid flows in bearings, coatings, and molds, and gas flows between rigid or elastic surfaces. To enable further applications of efficient, reduced-order modelling, we pursue streamlined algorithms for non-Newtonian liquids in marginally "thin" geometries with multiple phases and capillarity. The goal is expanded use of "modified", non-traditional lubrication methods to bring physics-based knowledge to bear in process design, optimization, and control methods.

Reynolds' lubrication applies to Newtonian fluids through thin flow channels. Accommodation for non-Newtonian flow behavior via generalized Newtonian constitutive relations can be achieved with the aid of variable transformations. The known stress-rate relation for a particular non-Newtonian rheological model can be transposed to yield pressure-drop/flowrate relationships of non-Newtonian lubrication flow. For non-moving boundaries, non-Newtonian lubrication can be formulated as one mass conservation and one momentum balance equation. When one or more channel boundaries are moving, the momentum balance expands to three equations to fully capture the shear-rate coupling between different momentum transport mechanisms.

For marginally high aspect-ratio flow channels, side walls exert significant drag on the flow that is not present in Reynolds' theory. An effectively lower liquid permeability instituted through a wall distance function suitably captures sidewall drag. Liquid-gas interfaces in filling applications are captured using level set tracking. Surface tension forces for high and medium Capillary Number flows are an additional lubrication modification. By combining an analytical thickness direction curvature with an in-plane level-set curvature field, wetting and de-wetting behavior are added to reduced-order lubrication modeling.

Non-Newtonian rheology, sidewall drag, and capillary forces are added to make a "modified" lubrication model. The resulting reduced dimensionality (3D flow problems are reduced to 2.5D) promises a "step change" in model efficiency leading to increased capability for model size and complexity. We demonstrate this reduced order method on the flow of Newtonian and power-law liquids through a patterned channel and find good agreement compared to a fully three-dimensional approach.

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Data-driven modeling and design of materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

REALISTIC RVES BY MICROSTRUCTURE RECONSTRUCTION: HARNESSING DESCRIPTOR DIFFERENTIABILITY

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ABSTRACT

One of the most important pillars supporting the digitization and acceleration of materials engineering is microstructure reconstruction and characterization (MCR). Specifically, MCR is needed for the following tasks: (i) creating a 3D computational domain that makes sense from 2D data, such as a microscopy image; (ii) reconstructing a small, periodic domain from a large, aperiodic CT scan; (iii) creating a set of statistical volume elements from a single reference; and (iv) enhancing microstructure datasets by sampling and interpolating in the descriptor space and then reconstructing the corresponding microstructures. The specific focus of this contribution is on descriptor-based MCR, in which the statistical microstructure description is given directly. Descriptor-based MCR has an advantage over machine learning-based MCR in that it does not need a data set. Instead, it can be used to create it, making data-driven modeling and simulation possible on otherwise insufficient amounts of data.

After a brief introduction to the underlying concepts, the potential of differentiable descriptors is analyzed in depth. As a first example, it makes the use of gradient-based optimization algorithms possible, reducing the number of iterations by orders of magnitude when compared to the Yeong-Torquato algorithm [1,2]. This is discussed alongside with a validation [3] and an implementation [4]. Secondly, this also applies to non-voxel-based structures, as is demonstrated by analytical solutions for ellipsoidal inclusions [5]. Thirdly, instead of solving a new optimization problem for each realization of a medium, a neural cellular automaton can be trained to identify a PDE system that generates structures very efficiently. Therein, the descriptors define the loss function and not data set us required. Finally, (approximate) gradient projection operators can be defined for individual descriptors, increasing the computational and memory efficiency even further.

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Advances in material model calibration for computational solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CALIBRATION OF HYBRID CONSTITUTIVE MODELS FROM FULL-FIELD DATA

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ABSTRACT

Constitutive models play a vital role in computational simulations, where they serve as closure relations for the general conservation laws of physics. Calibration is the process of estimating the parameters in a constitutive model from experimental characterization data. Generally, experiments provide indirect measurements of a material's response (e.g. applied force vs extension), which can only be directly related to constitutive model outputs in special circumstances (e.g. uniaxial stress in a tensile test prior to necking). In recent years there have been efforts to combine conventional constitutive models with machine learning (ML) components to produce hybrid constitutive models with the promise of increasing predictive accuracy and/or providing flexibility in the calibration process.

However, the scientific ML research community overwhelmingly favors training data in the form of direct constitutive model responses (e.g. stress-strain data from another model). This focus on direct measurements is stifling progress by divorcing ML models from their ultimate application within large-scale physics simulations and preventing the use of sources of experimental data that provide indirect measurements. These include infrared thermography and digital image correlation, information-rich metrology techniques for obtaining full-field temperature and deformation (i.e. displacement and strain) measurements, respectively, on the surface of a test specimen.

Furthermore, conventional constitutive models extrapolate in a manner that is well-understood and inherently stable. On the other hand, off-the-self ML models can extrapolate in undesirable, sometimes catastrophic ways. Robust extrapolation is crucial for constitutive models because characterization tests are limited by the design of laboratory equipment — they cannot impose arbitrary states of mechanical and/or thermal loading onto a material. Hence, in an application simulation, a constitutive model will surely extrapolate from the available data.

In this talk, we will discuss the structure of our hybrid models, training methods, and results obtained using synthetic and experimental full-field datasets.

New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZED-THERMAL CLOAKS FOR TRANSIENT HEAT CONDUCTION

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ABSTRACT

Thermal cloak is a metadevice that can realize thermal undetectability which is an analogy of optical invisibility and a thermal cloak, usually surrounding an insulating obstacle, reproduces temperature field without disturbance around the cloak as if no insulating obstacle is present. Thermal cloaks are usually composed of thermal metamaterials arranged based on transformation thermotics. Thermal metamaterials realize required thermal properties such as anisotropic thermal conductivity by tuning the artificial microstructures. Some different schemes have been also proposed based on isotropic bulk materials for thermal cloaking without using thermal metamaterials. A bilayer thermal cloak is composed of insulating and higher conductive layers whose widths are rigorously derived from the governing equation, thus it realize high performance in thermal undetectability despite its very simple structure.
Also, an ultrathin thermal cloak, that is the extension of the above bilayer scheme to three dimension, was proposed and was experimentally demonstrated. Topology optimization is one of the promising approach to design the thermal cloaks, level set and density-based optimum designs are numerically demonstrated. However, the above thermal cloaks are usually designed for steady state heat conduction.
In this study, an attempt is made to design a thermal cloak in transient heat conduction both to suppress the disturbance of outer temperature distribution and to reproduce the time variation of the temperature field from the initial state to the steady state in a transient heat conduction. To suppress the temperature disturbance caused by a thermal insulator, the difference between cloaked temperature and that without disturbance in transient state is minimized as the objective function. Radial Basis Function (RBF) parameterized-level set method is employed as a structural modeling to reduce the number of design variables without sacrificing the accuracy of finite element analyses. A covariance matrix adaptation evolution strategy (CMA-ES) is employed to explore the optimal set of design variables because of its robustness to difficult properties such as multimodality, interdependence between design variables, etc. CMA-ES is a multi-point search that adapts its distribution parameters for sampling, i.e. the shape, size and center of the distribution of candidate solutions generated based on normally distributed-random numbers. The use of CMA-ES makes designers free from guessing the appropriate initial solution and adjusting strategy parameters.

Multiscale modeling, analysis and numerical methods of material defect and inhomogeneities
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INVESTIGATION OF DIFFUSION BEHAVIOR AND ACTIVATION ENERGIES OF SELF-INTERSTITIAL ATOMS IN ALPHA-IRON USING MACHINE LEARNING INTERATOMIC POTENTIAL

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ABSTRACT

The neutron irradiation embrittlement of reactor pressure vessel steels is known to be caused by an extensive formation of point defects due to the neutron irradiation. The point defects spontaneously generate their clusters by their self-diffusion and affect significantly the generation and behavior of dislocations [1]. One of the typical point defects formed by neutron irradiation is the Self-Interstitial Atom (SIA) in which an extra atom is inserted between crystal lattices. The diffusion behavior and activation energy of SIA in α-iron have been extensively studied by atomistic computer simulations with either the first-principle calculations or empirical interatomic potentials. However, the activation energy of SIA diffusion calculated by empirical interatomic potentials differs from the result of first-principles calculations. Therefore the diffusion behavior and activation energy of SIA calculated by the empirical interatomic potentials are not reliable [2].

On the other hand, owing to the development of machine learning technique in computational engineering and science, interatomic potentials for α-iron have recently been developed by the machine learning technique, and it has been shown that they can reproduce the behavior of screw dislocations, which could not be reproduced by empirical potentials, with the same accuracy as first-principles calculations [3]. In this study, we aimed to confirm the reliability of the machine learning interatomic potential in the numerical simulation of the diffusion of SIA in α-iron. We calculated the activation energy and reaction pathways associated with the diffusion of SIA and compared the results with those obtained by existing interatomic potentials and first-principles calculations. As a result, the activation energies calculated by the machine learning interatomic potentials showed good agreement with the first-principles calculations for all diffusion mechanisms. Furthermore, the minimum energy paths were calculated, revealing that all diffusion mechanisms can be reproduced by the repetition of the diffusion mechanism with the minimum activation energy.

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Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CABANAPD: A MESHFREE GPU-ENABLED PERIDYNAMICS CODE FOR EXASCALE FRACTURE SIMULATIONS

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ABSTRACT

Peridynamics is a nonlocal reformulation of classical continuum mechanics suitable for material failure and damage simulation, which has been successfully demonstrated as an effective tool for the simulation of complex fracture phenomena in many applications. However, the nonlocal nature of peridynamics makes it highly computationally expensive, compared to classical continuum mechanics, which often hinders large-scale fracture simulations. In this talk, we will present CabanaPD, a meshfree GPU-enabled peridynamics code for large-scale fracture simulations. CabanaPD is built on top of two main libraries: Kokkos and Cabana, both developed throughout the Exascale Computing Project (ECP). CabanaPD is performance-portable and exascale-capable, and it is designed to run on U.S. Department of Energy’s supercomputers, including Frontier, which is the first exascale machine and today's top supercomputer worldwide.

Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ALGORITHMS FOR LOCAL-TO-NONLOCAL COUPLING AND ADAPTIVITY

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ABSTRACT

Many problems in computational mechanics involve the use of nonlocal models. Examples include molecular dynamics at the atomistic scale and peridynamics at the continuum scale. Simulations based on these nonlocal models normally involve computations between particles and large neighborhoods, making them significantly more computationally expensive than simulations based on classical (local) partial differential equations (PDEs). A balance between numerical accuracy and computational cost can be attained by coupling local and nonlocal models, where nonlocal models are used where required, for example in regions where cracks develop, while classical PDEs are employed elsewhere in regions where the assumptions of classical continuum mechanics remain valid; in the case of molecular dynamics, such methods are referred to as atomistic-to-continuum (AtC) coupling methods. AtC coupling is a special case of local-to-nonlocal (LtN) coupling. In this presentation, we will provide an overview of LtN coupling methods, focusing on peridynamics, and discuss adaptive strategies for application to fracture simulations.

MULTIFIDELITY LINEAR REGRESSION VIA A COMBINED LOSS FUNCTION FOR DATA-CONSTRAINED APPLICATIONS

Vignesh Sella[*1], Anirban Chaudhuri[1] and Karen Willcox[1]*

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ABSTRACT

Many-query tasks in science and engineering, such as uncertainty quantification, design optimization, and sensitivity analysis, involving an expensive-to-evaluate model are typically computationally prohibitive. One class of methods for reducing computational cost is by building surrogates, such as linear regression, for approximating the high-fidelity model outputs. However, accurate surrogate modeling remains a challenge for applications with limited training data. In this work, we develop a multifidelity linear regression method for applications where the capacity for high-fidelity data generation is significantly constrained. Typically, multifidelity surrogate models utilize multiple loss functions and combine the outputs of each underlying approximation via some model management technique, such as in the Kennedy-O'Hagan approach [1]. In contrast, the proposed work explores ways to create a single loss function for linear regression that combines many training data points from multiple low-cost, lower-fidelity information sources with few training data points from the high-fidelity source. One way to use a combined loss function is through weighted linear regression, where lower-fidelity models are assigned different weights as shown in Ref. [2]. The multifidelty setup also allows for the ability to fit higher-order polynomials by fitting one regression model that can utilize the larger sample pool available from the lower-fidelity models along with the high-fidelity data in a single training phase.

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Data-driven modeling and design of materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE MODELLING OF STRONGLY HETEROGENEOUS MATERIALS USING GEOMETRY INFORMED CLUSTERING

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ABSTRACT

Heterogenous materials such as 3D woven composites are designed with yarns traversing in-plane and through the thickness. This internal material architecture provides an improved performance in transverse loading conditions. However, the materials and manufacturing induced heterogeneity originating from the yarn crimp, waviness, non-uniform levels of compaction and the associated localised deformations results in a significant challenge in modelling these mesoscale features at structural length-scales. Although the material architecture lacks periodicity, it is repetitive [1]. To enable modelling at larger length-scales, a multiscale method that identifies clusters within the internal material architectures to find the repetitive patterns in the mesoscale and perform macroscale computations using these patterns is developed [2]. 3D Voronoi cells are used as the geometric entities in the material clusters, since Voronoi cells tessellates the unit-cells and function as the building blocks of the woven material architecture. Using k-means clustering, the mesoscale woven architectures are clustered offline and stored along with their constitutive data. This data is stored in a kd-tree structure to enable fast searches across the database. When online macroscale computations are performed, an intermediate stage correlation modelling is performed using 3D image registration, which compares the data clusters not only in terms of geometry but also against the material property stored in the voxels. The rigid transformation used in this registration retains the material objectivity. Using a predefined correlation criterion, data clusters are retrieved from the database and online computations are performed without explicitly modelling the mesoscale material architectures. The steps of this multiscale framework are verified and validated with different examples. A three-point bending problem is modelled to demonstrate how macroscale computations can be performed with few Voronoi clusters and the corresponding ability to model shear dominated regions. Additionally, a twill weave material architecture, unknown to the framework before the start of the analysis, is also analysed. Overall, this method results in a 45% reduction in computational cost whilst retaining the numerical accuracy which is verified by comparing the element-wise error histograms in stress and strain against mesoscale models.

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Data-driven approaches for solid mechanics
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INCREMENTAL NEURAL CONTROLLED DIFFERENTIAL EQUATIONS FOR PATH-DEPENDENT MATERIAL BEHAVIOR

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ABSTRACT

Data-driven surrogate modeling has emerged as a promising approach for reducing computational expenses of multiscale simulations. Recurrent Neural Network (RNN) is a common choice for modeling of path-dependent behavior. However, previous studies have shown that RNNs fail to make predictions that are consistent with perturbation in the input strain, leading to potential oscillations and lack of convergence when implemented within finite element simulations. In this work, we leverage neural differential equations which have recently emerged to model time series in a continuous manner and show their robustness in modeling elasto-plastic path-dependent material behavior. We develop a new sequential model called Incremental Neural Controlled Differential Equation (INCDE) for general time-variant dynamical systems, including path-dependent constitutive models. INCDE is formulated and analyzed in terms of stability and convergence. Surrogate models based on INCDE are subsequently trained and tested for J2 and Drucker-Prager plasticity. The surrogate models are implemented for material point simulations and boundary value problems solved using the finite element method with various cyclic and monotonic loading protocols to demonstrate the robustness, consistency and accuracy of the proposed approach.

Physical models and reduced order models augmentation with data for physics-informed machine learning in real-world applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NOVEL INTEGRATION OF 1D BLOOD FLOW EQUATIONS WITH PHYSICS-INFORMED GRAPH NEURAL NETWORKS FOR ARTERIAL PULSE WAVE PROPAGATION PREDICTION WITH IN VIVO VALIDATION

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ABSTRACT

Using computational models serve as predictive tools for hemodynamic parameters, contribute to optimizing surgical plans, and improve our understanding of cardiovascular diseases. With increasing demand, researchers often seek for machine learning methods that capture key dynamics without overloading computational resources and with less clinical measurements.

In this study, we propose a method that synergistically integrates 1D blood flow equations with Physics-Informed Graph Neural Networks (PIGNNs) to estimate the propagation of blood flow velocity and lumen area pulse waves along human systemic arteries. Our methodology involves the creation of a graph based on arterial topology, where each 1D line represents edges and nodes in the blood flow analysis. The innovation lies in decoding the mathematical data connecting the nodes, where each node has velocity and displacement of lumen area waveform outputs. The training protocol for PIGNNs involves measurement data, specifically velocity waves derived from inlet and outlet vessels and diastolic lumen area measurements from each vessel. To optimize the learning process, our approach incorporates fundamental physical principles directly into the loss function. This comprehensive training strategy not only harnesses the power of machine learning but also ensures the PIGNNs respect fundamental laws governing fluid dynamics, resulting in a model that is not only data-driven but also physically grounded.

The proposed methodology's accuracy was tested in silico and in vivo for various arterial topologies, in silico models containing idealized aortic bifurcation and pelvic topologies with 7 vessels with 3 bifurcations. In such models, we obtained a wave similarity coefficient of determination (R2) with conventional 1D blood flow models, and PIGNNs prediction consistently exceeded 0.99. In vivo models, particularly mouse carotid and aortic bifurcations, showed a R2 greater than 0.90 and root mean square error for diastolic and systolic lumen area values less than 10^(−10) .

This research marks a significant advancement, showcasing the ability to calculate lumen area and blood flow rate in all vessels within a given topology by seamlessly integrating 1-D blood flow with PIGNNs, using only blood flow velocity measurements. Moreover, this study is the first to compare the PIGNNs method with other classic Physics-Informed Neural Network (PINNs) approaches for blood flow

simulation. Our findings highlight the potential to use this cost-effective and proficient tool to estimate real-time arterial pulse waves.

Data-driven modeling and design of materials
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MICROMECHANICAL PROPERTIES PREDICTION OF MULTIPHASE FRP COMPOSITES USING CNN APPROACH

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ABSTRACT

A novel micromechanical characterisation technique is presented to predict the elastic modulus and failure initiation stress of two-phase fibre reinforced plastic (FRP) composites using the convolution neural network (CNN) technique. The proposed methodology can predict the stress-strain behaviour of a given microstructure under uniaxial tension or compressive loads. Macroscale properties of advanced FRP composites highly depend on the microscale arrangements, geometry and properties of the constituents. Current research on composite materials in the literature is heavily focussed on developing high-performance structural composites using highly toughened matrix materials with multifunctional capabilities. These new generation matrix materials exhibit a highly nonlinear behaviour under different loading conditions [1]. Mechanical characterisation of multi-phase materials is tedious due to the nature of diverse parameters controlling the effective properties, for example, manufacturing parameters and constituent properties. The phase materials, for example, toughened polymer matrices exhibit distinct deformation and failure behaviours under uniaxial loading conditions. Therefore, we propose a surrogate methodology to generate the stress-strain curve of the microstructures using statistical quantification followed by CNN.

A random fibre packing algorithm including the edge periodicity is employed to generate RVE of the microstructures comprising 40-70 % fibre volume fractions. Progressive damage analysis of the RVEs under tension and compression has been carried out using calibrated elastoplastic material models implemented in Abaqus/Explicit as a VUMAT user material subroutine. Homogenised stress-strain curves are then derived from the results of the elastoplastic RVE analyses. The generated RVE images and their corresponding stress-strain curves, constituting the dataset, are used to train the selected neural network architecture, i.e., CNN. The dataset comprises 2800 RVEs of various volume fractions are utilised for the study. The dimensions of the structure-property data are reduced by principal component analysis (PCA) technique before being fed into the CNN [2]. CNN models were then trained to accurately predict the elastic modulus, stress data at damage initiation and maximum stress before failure of FRP microstructures, with prediction errors of less than 10%. The proposed strategy can be used to design multi-phase microstructures and predict their non-linear stress-strain responses with better accuracy and minimal computational effort.

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OPTIMIZATION OF RESISTANCE PERFORMANCE BY ALTERING THE SHAPE AND POSITION OF SKEGS FOR THE TRANSPORTATION BARGE

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ABSTRACT

Appendages attached to the ship are used for stationkeeping, maneuvering, and motion performance. However, these appendages can increase the resistance of ship, so they must be carefully considered in design and engineering stages. In particular, for the transportation barge, skeg is installed on the stern to ensure course stability during towing. As the size of skeg increases, course stability improves, but friction resistance increases as the wetted surface area of the barge increases. Therefore, optimization of the shape of skeg is required. In the present study, the optimization is performed by altering shapes of skegs on transportation barges. The position and shape of skegs are chosen as the design variables. The resistance of the barge and wetted surface area of skegs are considered as the objective function and the constraint variable, respectively. The resistance of the barge is derived using computational fluid dynamics (CFD), and the SHERPA(Simultaneous Hybrid Exploration that is Robust, Progressive and Adaptive) technique is employed for the optimization of the shape of skeg. As a result, the optimized skegs with improved performance of resistance are achieved. The developed optimization procedure is expected to be applicable to other ship appendages in the future.

Acknowledgments
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Multiphysics and data-driven modeling for cardiovascular biomedicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTIPHYSICS COMPUTATIONAL MODELING OF INTRA-ANEURYSMAL THROMBOSIS BY FLOW DIVERTER STENTS

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ABSTRACT

Flow diversion is a less invasive endovascular treatment for cerebral aneurysms. In the procedure, flow-diverter stents are placed in the parent artery at the level of the aneurysm neck to alter intra-aneurysmal blood flow, causing stasis and progressive intra-aneurysmal thrombosis. Subsequent occlusion of the aneurysm by thrombosis decreases the chances of aneurysm rupture. The intra-aneurysmal thrombosis and subsequent occlusion of the aneurysm depends on several factors including the shape and curvature of the parent vessel, the hemodynamic conditions of the parent vessel, the size and shape of the aneurysm, and properties of the flow diverter stent. The choice of appropriate flow diverter stent for the given morphology and hemodynamic conditions of the aneurysm is therefore important for a better outcome. Currently, device selection for this procedure depends heavily on the expertise of clinicians. High fidelity computational modeling and prediction of the effects of flow diverter stents on the hemodynamics and thrombosis in the cerebral aneurysms can provide valuable information for proper device selection. In the present study, we propose a patient-specific, multiphysics computational modeling of intra-aneurysmal thrombosis caused by flow diverter stents. Hemodynamics in the parent vessel and aneurysm is simulated by an incompressible, immersed boundary flow solver and the stent is modeled by immersed structures with line elements. Flow mediated thrombus formation is modeled by the coupled convection-diffusion-reaction equations for thrombin, fibrin, and platelets. Several different patient specific cases with various stent parameters are considered and the simulation results are discussed in terms of flow diversion and thrombosis effectiveness.

Mathematical modeling and simulation for social, environmental, and disaster prevention issues
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT OF A COMPUTATIONAL FLUID DYNAMICS MODEL FOR PREDICTING CO2 CONVERSION EFFICIENCY IN COKE OVENS

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ABSTRACT

The steel industry, a significant contributor to global CO2 emissions, faces the challenge of reducing its carbon footprint while maintaining production efficiency. One promising approach to mitigate this issue is the reuse of CO2 in coke oven gas. However, the experimental assessment of CO2 reduction potential in this context is costly and complex. Addressing this challenge, our study introduces a novel Computational Fluid Dynamics (CFD) model integrated with chemical reaction processes to predict the CO2 conversion efficiency in real coke ovens.

This research primarily focuses on the development and application of a CFD model that simulates the chemical and physical interactions in coke ovens, particularly the conversion of CO2. Our model incorporates complex chemical reactions associated with CO2 and coke oven gas, providing a detailed analysis of the gas dynamics and reaction kinetics. By simulating these processes, the model predicts the efficiency of CO2 conversion under various operational conditions, offering valuable insights into the optimization of this process.

A critical aspect of our study is the validation of the CFD model's predictions. We conducted a comprehensive comparison between the model's output and experimental data obtained from real-world coke oven operations. This comparison demonstrated a high degree of accuracy in our model's predictions, thereby establishing its reliability and effectiveness in estimating CO2 conversion efficiency in the steel production process.

By providing a cost-effective and accurate tool to predict CO2 reduction in coke ovens, our study opens up new avenues for the steel industry to mitigate its environmental impact. The CFD model can be adapted to various coke oven designs and operational settings, making it a versatile tool for iron and steel manufacturers worldwide.

In conclusion, our research contributes significantly to the field of environmental sustainability in the steel industry. By leveraging advanced CFD modeling techniques, we offer a practical solution to reduce CO2 emissions, thereby supporting the industry's transition towards more sustainable practices. Our findings hold the potential to revolutionize the way CO2 emissions are managed in the steel production process, marking a critical step towards a greener and more sustainable future.

Analytical models for nonlinear dynamics and evolved dynamics in natural, social and engineering sciences
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DETERMINATION OF HIGH-ORDER FREQUENCY RESPONSE OF NONLINEAR SYSTEMS USING THE ARC-LENGTH METHOD

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ABSTRACT

While linear systems have been extensively studied in the past few decades, they alone are often not precise enough to accurately describe the behavior of systems with strong nonlinearities. However, solving nonlinear equations usually demands an exponential increase in processing capacity and time when compared to their linear counterparts. As computers become more powerful, significantly more advanced nonlinear systems can be studied and analyzed, providing solutions that are more accurate for real-world applications.

When it comes to frequency analysis, nonlinear frequency response may show the phenomena of hardening or softening. In this case, the resonance peaks of the frequency response are tilted to the right or left, respectively, in comparison with the linear frequency response. The consequences of these phenomena might prove essential to the safety assessment of real-life structures as the resonance peak might greatly differ from those obtained in a linear analysis.

In this study, the high-order frequency response of the Helmholtz-Duffing oscillator is analyzed to evaluate its influence on the system. The oscillator exhibits symmetric nonlinearity represented by a cubic stiffness and asymmetric nonlinearity represented by a quadratic stiffness. The high-order harmonic balance method was used to determine the dynamic equation in the frequency domain. The nonlinearities were numerically integrated based on the coefficients of the Fourier series. Originally used to find the solution path of nonlinear static structural analyses, the arc-length method was adapted to determine the nonlinear frequency response.

The equations from the first-order harmonic balance method assume that the nonlinear system response, as well as the nonlinear forces, are dominated by the fundamental harmonic. In this case, high-order harmonics are neglected. When it comes to high-order frequency response, multiple harmonics are considered in the system response and the equations are derived from the high-order harmonic balance method. This study shows that the behavior of systems with cubic stiffness only is usually very accurate with the first-order analysis. However, when quadratic stiffness is present, multiple harmonics must be taken into consideration to accurately describe the system behavior. Otherwise, the frequency response is possibly inaccurate and sometimes chaotic, as it is not entirely dominated by its fundamental harmonic.

ON MODELING MICRO-SCALE STRAIN GRADIENT ELASTIC ADHESIVELY BONDED JOINTS

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ABSTRACT

As a bonded structure scales down to the microscale, the role of the adhesive joint becomes more relevant concerning the overall performance of the microdevice. At the small scale, the microstructural and size-dependent properties of thin adhesives start to play a key role in the mechanical response of the layered assembly [1]. The present work focuses on the derivation of a soft imperfect interface law in a composite, constituted by two solids, separated by a thin adhesive layer in the framework of strain gradient elasticity. The model is obtained by means of the asymptotic methods. The contact laws, expressed in terms of the jumps and means values of the displacements, normal derivatives of the displacements, represent a formal generalization of the soft elastic interface conditions [2]. The present study reveals the stiffening behaviors of layered structures and size-dependent phenomena, typical of micro-scale structures [3].

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PERFORMANT LOW-ORDER MATRIX-FREE FINITE ELEMENT KERNELS ON GPU ARCHITECTURES

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ABSTRACT

Numerical methods such as the Finite Element Method (FEM) have been successfully adapted to utilize the computational power of GPU accelerators. However, much of the effort around applying FEM to GPU's has been focused on high-order FEM due to higher arithmetic intensity and order of accuracy. For applications such as the simulation of subsurface processes, high levels of heterogeneity results in high-resolution grids characterized by highly discontinuous (cell-wise) material property fields. Moreover, due to the significant uncertainties in the characterization of the domain of interest, e.g. geologic reservoirs, the benefits of high order accuracy are reduced, and low-order methods are typically employed. In this study, we present a strategy for implementing highly performant low-order matrix-free FEM operator kernels in the context of the conjugate gradient (CG) method. Performance results of matrix-free Laplace and isotropic elasticity operator kernels are presented and are shown to compare favorably to matrix-based SpMV operators on V100, A100, and MI250X GPUs.

Continuum biomechanics of active systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PRECISION THERMAL THERAPY IN MULTI-LAYER SKIN TISSUE: MODELING WITH DISTINCT ABSORPTION-EXTINCTION UNDER INFRARED LASER IRRADIATION

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ABSTRACT

Laser therapies embody cutting-edge advances in non-invasive medical techniques. This study concentrates on enhancing precision thermal therapy by investigating the intricate interplay between laser radiation and the complex layers of human skin. Our method involves representing the skin as three layers —epidermis, dermis, and subcutaneous tissue—and strategically manipulating a range of wavelengths. We explore the subtle workings of absorption and extinction coefficients, with a specific focus on unraveling the scattering dynamics between these layers. The purpose of this research is to advance the development of thermal therapies, facilitating precise targeting of tissue depths.
To simulate heat distribution in multilayered skin tissue, we use a stepwise Heaviside Function to outline thermal and optical properties. We also incorporate a three-phase lag model to capture the time-dependent aspects of heat transfer. The solution to the governing equation, obtained via numerical simulation, indicates the possibility of selecting optimal laser wavelengths and characteristics. This approach enables us to attain desired temperatures at precise depths within the tissue, advancing our comprehension of customized thermal interventions in medical procedures involving laser technology.

Computational mechanics of soft matter and machines
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EMERGENT NETWORK MORPHOLOGY IN SOFT MATERIALS: FROM BIOLOGICAL TO ROBOTIC SWARMS

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ABSTRACT

The allure of soft materials, characterized by low density, substantial deformability, and customizable properties, has captivated engineers. Conventional top-down engineering approaches face challenges in achieving intricate macroscale behaviors. In this work, inspired by biological bottom-up strategies, we delve into the concept of emergence, observing how internal networks in slime molds and fungi optimize transport, solve mazes, detect masses, and memorize periodic events. Our research presents a comprehensive theoretical and computational framework elucidating the interplay between macroscopic features and localized tuning of mechanical properties, resulting in an emergent and coordinated response in network morphology. To achieve high-fidelity simulations in three-dimensional space, we propose incorporating a phase-field scalar variable for network matrix evolution and a diffusive-advective process for nutrient distribution. This approach is particularly challenging due to the intricate interplay of coupled physics, high-order partial differential equations, and the evolving complexity of geometry. Upon grasping these fundamental principles, we employ neural networks to transfer knowledge gleaned from simulations, generating substantial data. This knowledge transfer plays a pivotal role in developing a cyberphysical system integrating robotic swarms, marking the convergence of theoretical insights with practical applications in soft material engineering.

Nanomechanics and nanoscale thermal transport for new materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ENHANCEMENT OF POWER FACTOR THE CONVERSION OF WASTE HEAT TO ELECTRICITY BY NANO-ENGINEERING OF THERMOELECTRIC CHALCOGENIDE MATERIALS

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ABSTRACT

Innovative transport mechanisms are the fountain of youth of TE materials research. In the past two decades, many potentially paradigm-changing mechanisms were identified, e.g., resonant levels, modulation doping, band convergence, classical and quantum size effects, anharmonicity, the Rashba effect, the spin Seebeck effect, and topological states. These mechanisms embody the current states of understanding and manipulating the interplay among the charge, lattice, orbital, and spin degrees of freedom in TE materials. Many strategies were successfully implemented in a wide range of materials. The electrical and thermal properties of the doped Tellurium Telluride (Tl10Te6) chalcogenide nano-particles are mainly characterized by a competition between metallic (hole doped concentration) and semi-conducting state. We have studied the effects of Sn doping on the electrical and thermoelectric properties of Tl10-xSnxTe6 (1.00 ≤x≤ 2.00), nano-particles, prepared by solid state reactions in sealed silica tubes and ball milling method. Structurally, all these compounds were found to be phase pure as confirmed by the x-rays diffractometery (XRD) and energy dispersive X-ray spectroscopy (EDS) analysis. Additionally crystal structure data were used to model the data and support the findings. The particles size was calculated from the XRD data by Scherrer's formula. The EDS was used for an elemental analysis of the sample and declares the percentage of elements present in the system. The thermo-power or Seebeck co-efficient (S) was measured for all these compounds which show that S increases with increasing temperature from 295 to 550 K. The Seebeck coefficient is positive for the whole temperature range, showing p-type semiconductor characteristics. The electrical conductivity was investigated by four probe resistivity techniques revealed that the electrical conductivity decreases with increasing temperature, and also simultaneously with increasing Sn concentration. While for Seebeck coefficient the trend is opposite which is increases with increasing temperature. These increasing behavior of Seebeck coefficient leads to high power factor which are increases with increasing temperature and Sn concentration except For Tl8Sn2Te6 because of lowest electrical conductivity but its power factor increases well with increasing temperature.

Keywords: Sn doping in Tellurium Telluride nano-materials, electron holes competition, Seebeck co-efficient, effects of Sn doping on Electrical conductivity, effects on Power factor,

Multiscale methods for advanced manufactured materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPLORING THE APPLICATION OF MIXED SOLVENTS IN LIQUID-PHASE EXFOLIATION OF GRAPHITIC CARBON NITRIDES WITH MOLECULAR DYNAMICS

Ehsan Shahini[*1], Narendra Chaulagain[1], Karthik Shankar[1] and Tian Tang[1]*

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ABSTRACT

The quest to optimize the liquid-phase exfoliation (LPE) of graphitic carbon nitrides (g-C3N4) is critical for their application in nanotechnology. This study delves into the intriguing effects of mixed solvent systems on LPE. Based on a machine learning (ML) model developed in our prior research for single solvents [1] and using the simple rule of mixture, the free energy of exfoliation (ΔGexf) is predicted for a vast array of 200 solvent mixtures, each at a 50:50 volume ratio. Molecular dynamics simulations involving umbrella sampling and potential of mean force evaluations are performed to calculate ΔGexf for the mixed solvents, and the results are compared with the ML model prediction. Interestingly, our findings unveil that some systems deviate from the model prediction, suggesting synergy or antagonism between the two solvents in the binary mixture. In some systems, for example N-Methyl-2-pyrrolidone (NMP): Cyclohexane (CH), the efficacy of LPE is akin to the solvent with lower ΔGexf, indicative of better performance. While in some other systems, for example methanol (MET): Dichloromethane (DCM), the efficacy of LPE aligns with the solvent exhibiting higher ΔGexf, indicative of poorer performance. Our computational analysis and experimental investigations converge on the nuanced behavior of these mixtures, reinforcing the insights into solvent behavior and interactions during LPE. This study not only provides a thorough understanding into the molecular interactions driving solvent performance but also establishes a robust computational framework complemented by experimental verification. This approach opens avenues for the rational design of solvent mixtures to optimize exfoliation processes, crucial for the scalable production of two-dimensional materials.

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TAILORED THERAPY: ADVANCING CANCER CARE WITH QUANTITATIVE SYSTEMS PHARMACOLOGY AND DIGITAL TWINS

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ABSTRACT

The development of a digital twin (DT) for cancer offers a groundbreaking approach to foreseeing the progression of an individual's cancer by simulating each tumor's unique attributes and its response to treatments. Leveraging recent advancements in computational methods, our approach integrates mechanistic modeling, machine learning, and stochastic techniques to construct a comprehensive DT platform. This platform harnesses a wide array of data, including biological, biomedical, and electronic health records (EHR), to generate personalized predictions.

A key component of our strategy is the integration of machine learning methods with mechanistic models grounded in quantitative systems pharmacology (QSP), a commonly used computational method for evaluating dose-response relationships in drug discovery and testing. However, a significant hurdle in QSP modeling is the accurate estimation of parameters. Traditional mechanistic models often operate under the assumption of uniformity across patients' diseases, leading to parameter calibration based on heterogeneous data sources.

To craft a truly personalized DT, we focus on utilizing individual patient data for parameter estimation, sensitivity analysis, and uncertainty quantification. For each patient, we tailor the QSP model parameters using their specific data. Through extensive multi-dimensional sensitivity analysis and uncertainty quantification, we identify crucial interactions within the model and establish confidence intervals for predictions. This personalized QSP model, enriched with data-driven insights into cellular and molecular interaction networks, ultimately enables us to predict the trajectory of cancer evolution in response to targeted therapies, marking a significant stride in personalized cancer treatment.

Smart structures – Modelling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NON-LINEAR, RATE-INDEPENDENT MODEL OF FERROELECTRICITY

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ABSTRACT

This work aims to establish a rate-independent non-linear model of ferroelectricity. The model is based on a phenomenological and continuum mechanical approach, to effectively account for switching phenomena and electrical hysteresis in ferroelectric materials. The switching phenomenon is due to an irreversible polarisation, occurring beyond a certain threshold value of the electric field, which can be reversed by changing the direction of the applied electric field. As a result, when a cyclic electric field is applied, a ferroelectric polarisation-electric field hysteresis loop is observed [1,2].

Inspired by the general methods of classical plasticity [3], we defined a yielding surface, such that states inside the surface have reversible behaviour and states on the surface can attain irreversible behaviour. Whether a state on the yielding surface is irreversible depends on the time derivative of the yielding function, the proposed evolution law for the irreversible polarisation, and the values and evolution laws of the hardening variables, i.e., isotropic and kinematic hardening. The isotropic hardening increases the threshold for irreversible behaviour (the electric field associated with the first yielding polarisation), whereas the kinematic hardening moves the centre of the yielding surface. The Kuhn–Tucker complementarity and consistency conditions are applied on the surface for loading/unloading circumstances.

The Finite Difference Method (FDM) and Finite Element Method (FEM) are utilised to illustrate the capability and the effectiveness of the proposed model in reproducing the non-linearity and electric field-polarisation hysteresis loop. These numerical methods are applied toa boundary value problem in which a cyclic electric potential was imposed on the boundary of the domain.

The FDM and FEM codes are run separately for solving the electric potential and electric field throughout the domain. In the interior, the electric potential and electric field are evaluated. The successive over-relaxation method is employed to find the electric potential and then the electric field is obtained by differentiation. Finally, the time behaviour of the yielding function and the polarisation field are evaluated. This model improves our previous work [1], and facilitates the development of a fully elastoplastic-ferroelectric model, which is our next goal.

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APPLICATIONS OF A MULTI-RESOLUTION AND MULTIPHASE MESH-FREE PARTICLE METHOD TO GRANULAR GRAVITY-DRIVEN FLOWS

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ABSTRACT

This paper applies a fully Lagragian and three-dimensional Mesh-free particle method to simulate landslides and the resulting impulsive wave. These phenomena represent one of the most serious geohazards and challenging gravities-driven flow. With the escalating impact of climate change likely to increase the frequency of such catastrophic events, developing accurate methods to comprehend the complex Multiphysics and predict tsunami-generated waves from landslides is imperative. The granular medium released undergoes significant deformation as it slides down, transferring high kinetic energy to the fluid medium upon impact. Traditional mesh-based methods struggle with these complex transitional flows, leading to mesh distortions and model instability.

To address large deformations, energy transfer, and strong fragmentation, a mesh-free multiphase particle method proves advantageous. Adopting a phase-dependent multi-resolution technique accommodates the varying length scales required for accurate representation of fluid and granular materials in complex multi-scale physics. Simulation scenarios encompass complete aerial landslides, submerged landslides, and partially submerged landslides and are validated against experimental tests conducted at the Polytechnique Montréal laboratory. The granular phase is modeled as a non-Newtonian flow mixture, considering different wetting stages.

Results from the three-dimensional multi-resolution and multiphase model align with experimental outcomes, attesting to its accuracy. This study emphasizes the suitability of the mesh-free particle method for capturing intricate dynamics involving granular material, deformations, and fluid interactions. The phase-dependent multi-resolution technique enhances the model's fidelity, making it a valuable tool for understanding and predicting the impacts of gravity-driven flows, especially in the context of increasing geohazards associated with climate change.

MOLECULAR DYNAMICS SIMULATIONS OF ICE GROWTH UNDER A STATIC ELECTRIC FIELD INDUCED BY TRANSMISSION LINES

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ABSTRACT

Icing accumulation on transmission lines and their insulating equipment poses a significant threat to power systems. Whilst the influence of unrealistic ultrahigh electric fields on supercooled water nucleation has been studied in earlier publications, there remains a critical gap in understanding the solidification mechanism under realistic electric fields; typically, around 105 V/m. It is therefore the objective of this study to uncover the reasons behind how static electric fields along distinct crystal planes catalyze ice growth and how they influence the resulting ice structure.

To achieve the above objectives, we embarked on extensive molecular dynamics simulations employing LAMMPS software. The TIP4P/Ice rigid water model was applied due to its proximity to the experimentally observed melting point. Long-range Coulombic interactions were computed employing the Particle-Particle Particle-Mesh method (PPPM) with a cutoff distance set at 0.8 nm. We focused out attention on two coexistence system: hexagonal ice-water and cubic ice-water; each comprising 432 and 576 water molecules, respectively. The liquid phase was associated with the secondary prism plane in both configurations. All simulations were performed at constant temperature (T) and under constant pressure (P) using the Nose-Hoover thermostat. The timestep of each simulation was taken to be 2 fs.

The radial distribution function was employed to analyze changes in the average structure of the system and ice structures are identified by the CHILL+ algorithm. The melting temperature, a critical factor affecting the degree of super cooling, was determined through the direct coexistence method. Distinct characteristics in the growing and melting processes of coexistence systems containing individual hexagonal and cubic ice were due to their unique anisotropic structures and growth modes.

Our molecular dynamics simulations reveal that the initial state of the ice crystal structure significantly impacts the subsequent ice formation process. Specifically, in systems containing hexagonal ice and liquid water, no cubic ice existed. Conversely, hexagonal ice was generated in cubic ice coexistence systems. This illustrates that the transformation of cubic ice to hexagonal ice is irreversible. Additionally, there exists a correlation between the direction of the static electric field and the liquid-ice interface that influences the crystal phase transformations. The electric field could alter the dipole orientation of interfacial water molecules and further change the interfacial free energy. Ice crystals exhibit preferred growth along certain crystallographic planes, which have specific orientations or arrangements and hence are more susceptible to external electric field.

Fluid dynamics and SciML: Navigating challenges and seizing opportunities
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DIFFERENTIABLE PHYSICS FOR A-POSTERIORI LEARNING OF TURBULENCE CLOSURES

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ABSTRACT

Differentiable fluid simulators are increasingly demonstrating value as useful tools for developing data-driven models in computational fluid dynamics (CFD). Differentiable turbulence, or the end-to-end training of machine learning (ML) models embedded in CFD solution algorithms, captures both the generalization power and limited upfront cost of physics-based simulations, and the flexibility and automated training of deep learning methods. We develop a framework for integrating deep learning models into a generic finite element numerical scheme for solving the Navier-Stokes equations, applying the technique to learn a sub-grid scale closure using a multi-scale graph neural network. We demonstrate the method on several realizations of flow over a backwards-facing step, testing on both unseen Reynolds numbers and new geometry. We show that the learned closure can achieve accuracy comparable to traditional large eddy simulation on a finer grid that amounts to an equivalent speedup of 10x. As the desire and need for cheaper CFD simulations grows, we see hybrid physics-ML methods as a path forward to be exploited in the near future.

Machine learning algorithms for accelerating material characterization, discovery, design, and manufacturing processes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOWARDS CO-SOLVING FORWARD AND INVERSE BOUNDARY VALUE PROBLEMS IN SOLID MECHANICS USING CONCURRENT PINNS

Mostafa Sharifan[*1], Keith D. Humfeld[2], Milad Ramezankhani[1] and Abbas S. Milani[1]*

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ABSTRACT

Abstract: In the contemporary manufacturing era, marked by Industry 4.0, the utilization of deep learning models is fast gaining attention for comprehending and representing intricate systems due to their highly nonlinear nature. Integration of governing equations into such machine learning models, often termed as physics-informed learning, have become a powerful non-black box technique. It involves not only feeding input data into the learning model but also incorporating the fundamental equations that govern the physical behavior of the system. Unsupervised learning, in particular, demands consideration of such input-output governing equations. From an engineering applications perspective, in a typical forward boundary value problem, the objective is often to predict the system's behavior based on a given set of input variables. In an inverse problem, on the other hand, the challenge becomes determining the inputs that lead to a desired (often optimized) output, under prescribed constraints. In this study we discuss and exemplify the application of a new technique coupling multiple concurrent physics-informed neural networks (PINNs), each designed to address specific aspects of the forward and inverse problems in solid mechanics. By leveraging shared losses, these networks co-train collaboratively, harnessing the collective intelligence embedded in the data and governing equations. The approach holds promise in optimizing not only solid materials structures, but their manufacturing processes, especially in the face of data paucity.

Coupled computational mechanics: Solutions for FSI simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COUPLING OF AN ENRICHED BEAM MODEL WITH A COMPRESSIBLE FLOW MODEL FOR FLUID-STRUCTURE INTERACTION IN PIPELINES

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ABSTRACT

With the growing popularity of numerical modelling to ensure the safety measure in industry, the need of more accurate models is imminent. In particular, the numerical modelling of pipelines is under study in this work. The latter has often been conducted by the classical beam models that lack the kinematics of the cross-section of the tube structures. While, the use of shell elements in a three-dimensional model has improved the precision of the numerical studies, they have greatly increased the computational cost of the simulations. In this work, an enriched beam model has been employed [1]. The latter takes into account the variations of the cross-section by adding the shell kinematics to those of the classical beam model. A Fourier expansion is used for this purpose for which the number of cross-section modes can be truncated. The enriched beam model can particularly be useful in the fluid-structure interaction studies. Fluid transient events have traditionally been simulated using liquid single-phase flow models while the pipe wall motion is tackled by means of a one-dimensional beam model. The latter has been improved in the work of [2] who replaced the fluid model by a compressible two-phase flow based on the Homogeneous Equilibrium Model (HEM). In this work, the flexible tube structure is two-way coupled to the fluid using the previously mentioned one-dimensional beam model enriched with the kinematics of the cross-section shell elements. As it is done in [2], a finite volume and finite element approach were used for the resolution of the fluid and structure dynamics, respectively. Finally, the proposed coupled approach is assessed on water-hammer phenomena due to the damage they could cause the structure.

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Advances in numerical methods for solution of PDEs
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADAPTIVE REFINEMENT WITH FINITE TIME LYAPUNOV EXPONENTS IN LAGRANGIAN NUMERICAL METHODS

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ABSTRACT

Finite Time Lyapunov Exponents (FTLEs) measure the maximum stretching of infinitesimal Lagrangian volumes advected by a dynamical system within a specified (finite) time horizon. These exponents are calculated from the eigenvalues of the system's Cauchy-Green strain tensor. Typically, FTLEs are used to identify the most repelling or attracting materially invariant coherent structures in fluid flow. In this study, instead of their traditional use as a flow diagnostic tool, we use FTLEs to trigger remeshing in a Lagrangian numerical method (LNM). One benefit of LNMs is that they are inherently multi-scale, i.e., they naturally cluster numerical particles in the locations requiring largest resolution such as the high-gradient regions. However, the distortion of the underlying mesh connecting these Lagrangian particles requires remeshing after a certain time. Previous implementations of LNMs have relied on heuristics to trigger remeshing in both time and space. In a Lagrangian simulation, where the trajectory of each numerical particle is known, FTLEs can be readily calculated. We use FTLE fields to both trigger remeshing and spatially redistribute numerical particles while demonstrating the enhanced numerical efficiency across different flows on a sphere. FTLE-aided simulations can be run for longer times, allowing novel vortex breakdown mechanisms on the sphere to be revealed.

Architected materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FIBRO-POROUS ARCHITECTED HYBRID MATERIALS FOR MULTIFUNCTIONAL APPLICATIONS

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ABSTRACT

Our work showcases the fabrication of fibro-porous materials using additive manufacturing—a process that intertwines a fiber mesh within the open cells of a foundational porous scaffold. The technique we introduce achieves an integrated fiber mesh with finely tuned characteristics into the scaffold, bypassing the need for any post-manufacturing modifications. Utilizing a gyroid design for the base scaffold, we explore the emergent acoustic absorption, pressure drop, mechanical rigidity, and energy absorption qualities. Our findings, gathered through two-microphone normal incidence impedance tube assessments, demonstrate notable acoustic absorption enhancements in comparison to heavier, non-fibered porous materials, while also reducing weight by 33%. Additionally, measurements of pressure drop and airflow resistance suggest that the addition of fibers narrows pore size and augments flow resistance, thereby amplifying lower frequency sound absorption. We observe substantial reinforcement in mechanical attributes, with a 27% rise in stiffness and a 37.85% increase in yield stress. The energy absorption capacity per unit volume also increases by 30%, owing to heightened resistance against deformation. Our study confirms the significant multifunctional advantages of fibro-porous materials without a major weight penalty, paving the way for the creation of intricate, tailored engineering structures with specific functional requirements.

Trustworthy multi-fidelity and data-driven models for computational applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SYMPLECTIC MODEL REDUCTION OF HAMILTONIAN SYSTEMS USING DATA-DRIVEN QUADRATIC MANIFOLDS

Harsh Sharma[*1], Hongliang Mu[2], Patrick Buchfink[3], Rudy Geelen[4], Silke Glas[2] and Boris Kramer[1]*

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ABSTRACT

Classical symplectic model reduction approaches employ linear symplectic subspaces for representing the high-dimensional system states in a reduced-dimensional coordinate system. While these approximations respect the symplectic nature of Hamiltonian systems, linear basis approximations can suffer from slowly decaying Kolmogorov N-width, especially in wave-type problems, which then requires a large basis size. We present two novel approaches for the symplectic model reduction of high-dimensional Hamiltonian systems using data-driven quadratic manifolds. The addition of quadratic terms to the state approximation, which sits at the heart of the proposed methodologies, enables us to better represent intrinsic low-dimensionality in the problem at hand. The proposed approaches are effective for issuing predictions in settings well outside the range of their training data while providing more accurate solutions than the linear symplectic reduced-order models. Both of these novel approaches together constitute a first step towards the model reduction of dynamical systems on nonlinear manifolds using interpretable (e.g., polynomial) manifold constructions that ensure that the approximate solution satisfies key physical properties as dictated by the original high-dimensional problem.

Physics-based data-driven modeling and uncertainty quantification in computational materials science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A PHYSICS-CONSTRAINED POLYNOMIAL CHAOS FRAMEWORK FOR DATA-DRIVEN MODELING AND UNCERTAINTY QUANTIFICATION

Himanshu Sharma[*1], Lukas Novak[2] and Michael Shields[1]*

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ABSTRACT

Polynomial chaos expansion (PCE) is a widely adopted surrogate modeling method primarily employed for uncertainty quantification (UQ) of complex physical systems represented by expensive computational models. PCE has also recently been used as a machine learning (ML) method in a purely data-driven setting. PCE surrogate model is trained using a limited number of deterministic simulations from computationally expensive models and provides an efficient estimation of various output statistics, such as its moments and sensitivity to different stochastic parameters. However, ensuring an accurate approximation of the underlying model may require a considerable number of computationally expensive simulations, which is often challenging with physics-based models. To reduce the training data requirement, we can supplement the limited data with the known physics of the model, thereby improving the accuracy and computational efficiency. This necessitates a novel framework that incorporates physics knowledge through constraints in the PCE model. To this end, we develop a novel physics-constrained PCE surrogate model that can effectively incorporate a variety of physical constraints, such as initial and boundary conditions, governing partial differential equations, and inequality-type constraints (e.g., monotonicity, convexity, non-negativity). We demonstrate that integrating physical constraints enhances the accuracy of UQ assessment while requiring significantly fewer expensive simulations during the training process. Moreover, it ensures physically realistic predictions across the entire domain in data-driven modeling. This makes the proposed method ideal for UQ and ML applications involving physics-based models. We further proposed a sparse implementation that effectively reduces the number of polynomial basis needed to accurately capture the output response, thereby facilitating the use of the proposed method for high-dimensional problems.

UQ-TTA student paper competition in uncertainty quantification
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A PHYSICS-CONSTRAINED POLYNOMIAL CHAOS FRAMEWORK FOR DATA-DRIVEN MODELING AND UNCERTAINTY QUANTIFICATION

Himanshu Sharma[*1], Lukas Novak[2] and Michael Shields[1]*

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ABSTRACT

Polynomial chaos expansion (PCE) is a widely adopted surrogate modeling method primarily employed for uncertainty quantification (UQ) of complex physical systems represented by expensive computational models. PCE has also recently been used as a machine learning (ML) method in a purely data-driven setting. PCE surrogate model is trained using a limited number of deterministic simulations from computationally expensive models and provides an efficient estimation of various output statistics, such as its moments and sensitivity to different stochastic parameters. However, ensuring an accurate approximation of the underlying model may require a considerable number of computationally expensive simulations, which is often challenging with physics-based models. To reduce the training data requirement, we can supplement the limited data with the known physics of the model, thereby improving the accuracy and computational efficiency. This necessitates a novel framework that incorporates physics knowledge through constraints in the PCE model. To this end, we develop a novel physics-constrained PCE surrogate model that can effectively incorporate a variety of physical constraints, such as initial and boundary conditions, governing partial differential equations, and inequality-type constraints (e.g., monotonicity, convexity, non-negativity). We demonstrate that integrating physical constraints enhances the accuracy of UQ assessment while requiring significantly fewer expensive simulations during the training process. Moreover, it ensures physically realistic predictions across the entire domain in data-driven modeling. This makes the proposed method ideal for UQ and ML applications involving physics-based models. We further proposed a sparse implementation that effectively reduces the number of polynomial basis needed to accurately capture the output response, thereby facilitating the use of the proposed method for high-dimensional problems.

AN EFFICIENT BAYESIAN COMPUTATIONAL METHOD USING SCALABLE SOLVERS FOR STOCHASTIC PDES

Sudhi Sharma[*1], Ajay Kumar Verma[1], Pierre Jolivet[2], Victorita Dolean Maini[3] and Abhijit Sarkar[1]*

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ABSTRACT

The state or combined state and parameter estimation of extreme scale nonlinear stochastic computational models (generally arising from the discretization of stochastic PDEs), sampling based non-Gaussian filters (e.g. particle or ensemble Kalman filters) can become computationally impractical. To alleviate the computational challenges at the forecast (prediction) step of nonlinear filtering for such models, a two-grid scalable solver using (sampling-free) intrusive stochastic Galerkin method is developed that leverages two-level Schwarz method for geometric decomposition and the algebraic multigrid solver (AMG) for the corresponding coarse problem. This two-grid solver demonstrates scalable performance for high resolution spatial and temporal discretizations, a large number of input random variables and higher order stochastic (i.e. polynomial chaos) expansion terms for the output of nonlinear stochastic PDEs.

Within the framework of the polynomial chaos Kalman filter, the distributed implementation of the update (analysis) step will be developed that exploits this two-grid scalable solver to condition the system state using observational data. We will also investigate a specific case where only spatially averaged aggregated data in sub-regions are available. Such cases arise in the context of mechanistic geospatial modeling of infectious disease spread whereby the testing data for infected population averaged over public health units (defining a sub-region) are reported by public health agencies.

Geometric mechanics formulations and structure-preserving discretizations for continuum mechanics and kinetic models
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ON THE HAMILTONIAN STRUCTURE FOR A MODEL OF A CLOSED VORTEX SHEET AND A VORTEX PATCH IN AN IDEAL FLUID WITH A DENSITY JUMP

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ABSTRACT

The talk will discuss the Hamiltonian structure for the system of a closed vortex sheet dynamically interacting with a vortex patch in an ideal fluid. The equations of motion for a certain special configuration of this interaction, without reference to Hamiltonian form, was previously published with co-author Rangachari Kidambi. The closed vortex sheet separates an ideal fluid with two different densities, and the vortex patch is located either inside or outside the closed sheet. Following an introduction to vortex sheets and vortex patches, the talk will place this model in the framework of Hamiltonian fluid mechanics, in particular, in the modern symplectic mechanics framework of vortex dynamics.

Modern structure-preserving methods for PDEs
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN ADAPTIVE MOMENTS-BASED INTERFACE RECONSTRUCTION USING INTERSECTION OF THE CELL WITH ONE HALF-PLANE, TWO HALF-PLANES AND A CIRCLE

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ABSTRACT

We present a new adaptive moment-of-fluid (A-MOF) interface reconstruction method. It uses the zeroth, first, and second moments of the fragment of material inside a cell of the mesh to construct a shape that approximates the respective material fragment. The new method requires information about the material moments only for the cell under consideration. The adaptive method chooses between shapes obtained by the intersection of the cell with one half-plane, two half-planes, or a circle. The A-MOF method allows to exactly reproduce several convex shapes: corners, filaments, and their concave cell-complements; as well as pieces of the circles and its cell-compliments. Interface reconstruction is formulated as a local (for each cell), non-linear, equality constrained optimization problem, which does not require additional communication and allows for an efficient parallel implementation. In conclusion, we present an extensive set of test problems, both for interface reconstruction on a single cell, and for reconstruction of a variety of shapes on the entire mesh.

HYPOPTLIB: CRITICAL DESIGN INSIGHT INTO LARGE-SCALE DESIGN PROBLEMS IN TOPOLOGY OPTIMIZATION AND BEYOND

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ABSTRACT

Systematically understanding the solution space of large-scale design problems is crucial for answering a range of design questions, including sensitivity, performance, etc. These questions are particularly pressing for design problems where the answer depends on a large number of design variables, e.g., high-resolution problems in topology optimization. We present HypOptLib, a C++/Python code that implements novel filtration approaches to explore the solution space of large-scale design problems. Rather than merely seeking an optimized solution, HypOptLib yields detailed insight into the structure of the solution space, a capability often overlooked in conventional optimization libraries. HypOptLib exploits a mapping of design variables in conventional problems in topology optimization to the dynamics of pseudothermal systems of “particles.” We implement design variable dynamics by adapting techniques from molecular dynamics. Using compliance minimization as a demonstration problem, we demonstrate that HypOptLib supplements problems typically studied via topology optimization with critical insights into the reliability and sensitivity of design solutions. The problem-independent algorithm makes HypOptLib adaptable to a wide range of large-scale design problems in topology optimization and beyond where understanding.

MODELING DAMAGE AND HEALING OF DISORDERED POROUS MATERIAL WITH HOMOGENIZED MICROSTRUCTURE USING PERIDYNAMICS

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ABSTRACT

Microstructure geometry plays a crucial role in determining the mechanical behaviour of porous materials. In addition to porosity, the distribution of pores, which we quantify as disorder, is also a significant factor for these materials. Using artificially generated porous microstructures, it has been shown in previous studies[1] that the elastic modulus, peak strength and the work of failure of a porous material depends on the disorder. Similarly, peak stress and work of failure obtained from the simulations can be compared with findings by Kirsch[2], and considering multiple voids as equivalent to a single void. It is observed that for peak stress and work of failure, effect of disorder is even more pronounced than elastic modulus and for high disorder these values are much lower than as predicted by the mean field approach. At higher levels of disorder and porosity, probability of the existence of weak spots with high stress concentration increases, which causes a a knock-down effect. In the previous study, Peridynamics has been used to analyse the failure because of the ease with which it can capture damage and fragmentation. However, modeling porous microstructure in Peridyanmics comes with multiple caveats, such as the need for a very small discretization size to capture the geometrical details, leading to a small time step size for stability maintenance. This leads to very high computational costs and makes computation of large structures almost impossible. Therefore a homogenization technique is necessary in order to reduce the computational cost, without sacrificing the effects of microstructure geometry. To this end, the Intermediate Homogenization (IH) proposed by Chen et al.[3] has been used, where peridynamic bonds of a material point is deleted in a manner that the homogenized structure still carries some information about the microstructure, in our case porosity and disorder. In a similar fashion, bonds may also be created, to simulate healing of damaged structure. This technique is then used to simulate compression in snow, a process that undergoes both damage and healing. The results are then compared with experimental results.

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Data-driven approaches for solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICS-INFORMED MACHINE LEARNING MODEL FOR BRITTLE DAMAGE PREDICTION

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ABSTRACT

Physics-informed Neural Network (PINN) has been introduced recently to predict and understand complex physical phenomena by directly incorporating feedback from governing equations. While PINNs offer remarkable capabilities, challenges arise when addressing discontinuities and heterogeneity, potentially compromising accuracy and reliability in prediction outcomes. In this study, a novel approach that combines the principles of peridynamic (PD) theory with PINN is presented to predict quasi-static damage and crack propagation in brittle materials. To achieve high prediction accuracy and convergence rate, the linearized PD governing equation is enforced in the PINN's residual-based loss function. The proposed PD-INN is able to learn and capture complicated displacement patterns associated with different geometrical parameters, such as pre-crack position and length. The computational method presented in this study can be implemented to any PD constitutive model like Bond-Based PD or State-Based PD as well as any horizon factor. Several enhancements like cyclical annealing schedule and deformation gradient aware optimization technique are proposed to ensure the model would not get stuck in its trivial solution. The model's performance assessment is conducted by monitoring the behavior of loss function throughout the training process. The PD-INN predictions are also validated through several benchmark studies, with the results obtained from high-fidelity techniques such as the PD direct numerical method and the Extended-Finite Element Method. Our results show the ability of the nonlocal PD-INN to predict damage and crack propagation accurately and efficiently.

Microstructures of chemically complex materials and their impacts on material properties from multiscale simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TEMPERATURE-DEPENDENT ELASTIC PROPERTIES OF BORON CARBIDE FROM FIRST-PRINCIPLES CALCULATIONS AND PHONON MODELING

Sara Sheikhi[*1], Wylie Stroberg[1] and James Hogan[1]*

[1]*University of Alberta*

ABSTRACT

Advanced ceramics, like boron carbide, exhibit high chemical and thermal stability, and abrasion resistance. These outstanding properties make them suitable for applications in extreme conditions, including thermal barrier coatings, aerospace applications, and as neutron absorbers. Understanding the behavior of boron carbide in extreme conditions is pivotal for accurately predicting its mechanical properties, a crucial step in designing and optimizing next-generation materials. In the limited literature, density functional theory (DFT) and molecular dynamics (MD) simulations have been used for investigating the microstructure and mechanical properties of boron carbide. The estimation of Cij at elevated temperatures is largely unexplored, except for MD simulations; however, these simulations can lack sufficient accuracy in interatomic potentials at different temperatures, particularly in the context of single-crystal boron carbide. The boron carbide's unit cell consists of a 12-atom icosahedral cage surrounding a 3-atom linear chain along the (111) rhombohedral axis. The chemical similarity between boron and carbon induces substitutional disorder, resulting in different structures in the thermodynamic limit. The concentration of carbon in the structures can vary from 6.66% to 26.66%; this variability results in a complex phase diagram, challenging the study of boron carbide's mechanical and electronic properties. In this study, temperature-dependent Cij, thermal expansion coefficient (TEC), Helmholtz free energy, entropy, and heat capacity at constant volume (Cv) of boron carbides with different stoichiometries have been predicted using first-principles quasi-harmonic phonon calculations. A combination of first-principles volume-dependent calculations, and phonon calculations, has been performed. Good agreement between elastic constants and structural parameters from static calculations is observed. The thermodynamic properties from phonon calculations show trends that align with the literature. As the temperature rises, we observe a decrease in free energy, while entropy and Cv increase. The temperature-dependent TEC trend shows a minimal increase below 100K, followed by a sharp rise until 500-700K and then a gradual increase until it approaches a nearly constant value. This trend is attributed to the transition from internal energy dominance to vibrational entropy dominance, indicating significant changes in the material's behavior as temperature increases. Temperature-dependent Cijs are predicted, enabling stress analysis at elevated temperatures. Below 100K, elastic constants remain nearly constant due to minimal atom vibration. All elastic constants decrease with increasing temperature, except C44, which exhibits almost no change, emphasizing boron carbide's anisotropic behavior. Overall, this study's outcomes can be used in performing mechanical and thermal stress analysis and optimizing design of boron carbide materials for elevated temperature applications.

Advanced techniques for transport phenomena in heterogenous porous media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPERIMENTAL AND MOLECULAR SIMULATION STUDIES OF METHANE ADSORPTION ON DEEP SHALES

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ABSTRACT

Understanding methane adsorption behavior on deep shales is crucial for estimating the original gas in place and enhancing gas recovery in deep shale gas formations. However, the methane adsorption behavior on deep shales under high pressure is challenging, and many uncertainties still exist in the process. In this study, the methane adsorption on deep shales within the Lower Silurian Longmaxi Formation from the Sichuan Basin, South China were conducted at pressures up to 50 MPa. The effects of total organic carbon (TOC), temperatures, clay minerals and moisture content on the adsorption capacity were discussed. Then the molecular models of kerogen nanopores with different shapes and sizes were constructed based on kerogen structure unit of deep shale from the Longmaxi Formation, and the methane occurrence were conducted by coupling a grand canonical Monte Carlo algorithm and a molecular dynamics algorithm. The results indicated that the methane excess adsorption on deep shales increased, then reached its peak and finally decreased with the pressure. The methane adsorption capacities exhibited strong positive correlations with the TOC content and negative relationships with clay minerals. The methane excess adsorption decreased as the temperature while the opposite trend would occur once it exceeded some pressure. The presence of the moisture content on deep shales sharply decreased the methane adsorption capacities, and the reduction of the adsorption capacity decreased with the pressure. The methane adsorption capacity in deep shales is negatively correlated with temperature, and high temperature will inhibit the affinity of methane molecules in pores.

Multiscale modeling, analysis and numerical methods of material defect and inhomogeneities
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STABLE AND EFFICIENT METHODS FOR 2D-3C CLAMPED PLATE AND SHALLOW SHELL MODELS

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ABSTRACT

In this talk, we share our work on the numerical approximation for the two-dimensional three-component (2D-3C) clamped plate and shallow shell problems. The clamped plate and shallow shell structures are non-negligible in engineering, especially in architectural design, aerospace, and automated manufacturing. Therefore, it is crucial to develop efficient numerical algorithms to analyze their mechanical behavior accurately.

In solving such problems, we face two significant challenges. On the one hand, the complex variable coefficient system on the 2D surface complicates the discretization process. On the other hand, the displacement components have a high degree of regularity, further increasing the difficulty of discretization. We introduce discretization schemes of conforming, nonconforming, and virtual elements to meet these challenges. Moreover, the new contributions include well-posedness and stability for the approximate problem and analysis of the convergence of the numerical solution. Finally, numerical results show that the stability and convergence of the numerical schemes are verified.

CENTRAL WENO-ZN SCHEME WITH THE OPTIMAL ACCURACY ORDER AT HIGH-ORDER CRITICAL POINTS

Yiqing Shen[*1], Biao Zhou[1], Hao Jin[1], Yi Cheng[1] and Jianyu Qin[1]*

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ABSTRACT

The high order critical points (the first n-th derivatives equal to zero while the (n+1)-th one does not) measure the different scales structures in the complex flow fields. The shock-capturing schemes with the highest possible accuracy order at critical points are so desired for the delicate simulations of compressible flows, such as the large eddy simulation and the direct numerical simulation of compressible turbulence. One kind of weighted essentially non-oscillatory(WENO) scheme (WENO-ZN[1,2]) was recently proposed to improve the accuracy of WENO schemes by using a high-order global smoothness indicator and to keep the ENO-property by an adaptive function.

This paper develops the high-order central WENO-ZN (C-WENO-ZN) scheme by combining the ideas of the WENO-ZN and OWENO[3] schemes. Different to that of the previous WENO-ZN schemes, the smoothness indicator of each candidate stencil is calculated by the half-point formula, the global smoothness indicator is calculated by a simplified but more effective form(compared to that of OWENO), and a corresponding adaptive function is also constructed to enhance the ENO-property. Numerical results are present to show that the proposed C-WENO-ZN scheme can achieve high order convergence rate at critical points, is high robust for solving various complex flow fields, and also has other advantages such as the low dissipation and favorable symmetry.

Key words: Weighted essentially non-oscillatory scheme, Critical point, Optimal accuracy, Low dissipation, Symmetry.

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The phase field method for fracture: Theory, numerics, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN ACCELERATION SCHEME FOR THE PHASE FIELD FATIGUE FRACTURE SIMULATION

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ABSTRACT

The fatigue fracture brings severe mechanical failures. In recent years, the phase field approach for fracture has been extended to fatigue fracture. In this study, we propose an efficient acceleration scheme for the phase field approach based on a concurrent time-scale homogenization theory. In this scheme, the fatigue fracture problem is decomposed into a macrochronological problem and a microchronological problem, and is accelerated with the macrochronological time steps adaptively determined. Throughout the whole simulation, the macrochronological time step is monitored, and is corrected by a predictor-corrector strategy if necessary. This scheme is able to accelerate fatigue fracture simulations without sacrificing much accuracy, and can be up to 200 times faster than direct numerical simulations in some cases. For certain force-controlled examples, the proposed scheme, equipped with the arc-length control, is able to reproduce Paris' law with a correlation coefficient higher than 0.91 in the logarithmic scale.

Advanced materials: Computational analysis of properties and performance
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREDICTION OF WRINKLE PATTERNS IN THIN FILM-COMPLIANT SUBSTRATE SYSTEMS: DIRECT NUMERICAL SIMULATIONS

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ABSTRACT

Formation of wrinkles in thin-film structures has received considerable attention, due to their ubiquity in nature as well as in many modern devices in use or under development. It is a well-recognized form of deformation instability that can develop under mechanical or thermal loading. While wrinkling instability is frequently an undesirable feature, it has been increasingly exploited to create surface patterns with desirable optical, electronic, mechanical, or energy-harvesting functions. Depending on the loading condition and geometry, various 3D patterns and complex shapes may develop, the prediction of which is inherently challenging. In this presentation, we highlight our recent developments of a practical finite element based technique utilizing the embedded imperfections to trigger wrinkle formation. This approach leads to direct modeling from pre-instability to post-instability in a seamless manner, without the need of any cumbersome or multi-step procedure. It also gives new insights into the evolution of wrinkle patterns, and enables the prediction of global structural buckling which may coexist with surface wrinkles. Our studies include large-scale 3D simulations under general in-plane compression, spanning the entire biaxial spectrum in between the extreme cases of uniaxial and equi-biaxial loading. The effects of various material properties, deformation paths and loading sequences can also be analyzed, and the predictions can be correlated with experimental observations.

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A COMPARISON OF THE COMBINED-PARTICLE ELEMENT METHOD AND THE GENERAL PARTICLE ALGORITHM IN EPIC FOR APPLICATION TO CONCRETE PENETRATION

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ABSTRACT

Concrete is the most-produced manmade material in the world and is typically an integral component of U.S. military assets. These assets are designed to resist extreme impulsive loads such as those from blast or penetration. The ability to understand and predict terminal ballistic effects on concrete is crucial for the design and analysis of protective structures. Computational modeling of high-velocity impact problems like penetration and perforation have shown increased accuracy over the years as methods such as the finite element, finite difference, finite volume, and meshfree methods have continued to improve. One of the difficulties in modeling these impact events is capturing rapidly changing surfaces within the numerical framework. Meshfree methods offer an advantage in dealing with these rapidly changing surfaces, since they are unbounded by a fixed grid. However, meshfree methods experience an efficiency penalty due to determining the continuously evolving change of neighboring points, requiring the determination of neighbors on the fly. A solution to this problem has been the introduction of hybrid methods, which take the best qualities of both finite element and meshfree methods. Two hybrid methods exist within the EPIC (Elastic Plastic Impact Computation) code and are known as the General Particle Algorithm (GPA) and the Combined Particle-Element Method (CPEM) [1-2]. GPA has been used historically in the past to model high-velocity impact, while CPEM is a newer method offering greater accuracy than GPA. This study will evaluate both GPA and CPEM methods in their ability to accurately capture concrete penetration events. A sensitivity study will be performed, and the results will be compared to relevant experimental data.

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Applications of shape optimization in complex engineering problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SHAPE DESIGN OPTIMIZATION OF BIMETAL COMPOSITE STRUCTURES FOR DYNAMIC COMPLIANCE MINIMIZATION

Jin-Xing Shi[1] and Haruki Igawa*[1]

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ABSTRACT

Bimetals have been widely adopted and designed as parts or accessories in automobiles, aircraft, and marine engineering to meet specific requirements. Combining different material properties of two metals can generate new mechanical or physical behaviors.

The shape design optimization of bimetal composite structures plays a crucial role in achieving their optimal mechanical or physical performance. In our previous studies, we developed a gradient-based shape optimization method for composite structures with dissimilar materials, addressing stiffness maximization [1], thermal buckling [2], and control of vibrational eigenvalues [3] problems.

In industrial product design, vibration problems are critical and require careful consideration. Generally, vibration problems are classified into natural vibration, frequency response, and time response problems, with the time response problem being time-dependent and more complex than the other two.

In this study, we aim to extend the gradient-based method for shape design optimization of bimetal composite structures to address the dynamic compliance minimization problem, which falls under the time response category. The design problem is formulated as a distributed parameter optimization problem, and shape gradient functions, i.e. sensitivity functions, are theoretically derived for the shape variation to obtain the optimal interface and surface shapes of bimetals under two volume constraints for the different metals. The optimal results from numerical examples demonstrate that the dynamic compliance of bimetal composite structures can be significantly reduced by using the proposed shape optimization method.

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AN IMPROVED SECONDARY BREAKUP MODEL APPLIED TO WATER DROPPING OF FIRE-FIGHTING AIRCRAFT

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ABSTRACT

When water is released from the fire-fighting aircraft, a large amount of water splits up into fine particles and spreads in all directions affected by aerodynamics of water. It is essential to accurately simulate the process of aircraft dropping water and establish precise droplet aerodynamics analysis. Aiming at the complex multi-phase flow problem of water dropping, the process of aircraft water dropping is numerically studied based on Euler-Lagrange coupling method. In the initial stage of water release, the formation of ligaments and large droplets is simulated using the Volume of Fluid (VOF) method. The Euler liquid portion is converted to discrete Lagrangian drops according to empirical correlations and the droplet breakup model is used to calculate the secondary stage by Discrete Phase Model (DPM) method [1]. Comparing the droplet diameter distribution with the experimental results from the referenced study [2], the calculated results of existing breakup models show significant inconsistency with the experimental results. To address this disparity, an improved secondary breakup model in this paper, incorporating the wave breakup model and Madabhushi breakup model. Numerical calculations using the improved model reveal better alignment with experimental results in terms of droplet diameter distribution. This improved secondary breakup model offers a more accurate and efficient means of evaluating droplet diameter distribution. The method can quickly obtain more accurate droplet diameter distribution. The method provides a reliable calculation for the density distribution and impact load of water, which helps determine how to release water from a fire-fighting aircraft to extinguish a fire more efficiently.

Keywords: water dropping, secondary breakup model, VOF to DPM method

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Advanced materials: Computational analysis of properties and performance
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE MODELING STRATEGY FOR ACCURATELY PREDICTING FATIGUE LIFE OF STEELS

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ABSTRACT

This study presents a multiscale modelling strategy for accurately predicting the high-cycle fatigue strengths of steels. In the proposed strategy, total fatigue life is estimated from crack growth life alone based on the experimental facts.
The entire model comprises three sub-models, for: (i) a macroscopic finite element analysis, (ii) microstructure, and (iii) crack growth. The required input data are only microstructural information, tensile properties, and loading conditions, without any adjustable material constants. The aim of the model for (i) a macroscopic finite element analysis is to define an active zone where sufficiently contains the whole of possible crack initiation area and to obtain the strain amplitude field in the active zone. In the model for (ii) microstructure, we employed a modeling strategy with two steps of 2D problems, which is modeling for surface and inside of material considering the features of actual fatigue crack initiation and growth behaviors. The Monte Carlo method is applied to simulate distribution of the microstructure, which is a nature of the scatter of fatigue life. In the model for (iii) crack growth, we employed the interaction theory between crack and grain-boundaries. The driving force of the crack growth is quantified using crack tip sliding displacement (CTSD) formulated based on the continuously distributed dislocation theory considering slip transmission between adjacent grains. The material resistance of each phase is determined as the friction strength to move dislocations. All the grains assigned in the surface of the active zone are assumed as possible crack initiation sites and the number of cycles to failure is determined based on the weakest link assumption.
The model was strictly validated against the results of experiments performed on three different steels under various loading conditions using four types of specimens. Although the experimental fatigue life results exhibited wide variation, the predicted and experimental data were accurately matched over the entire range. The notch sensitivity of the fatigue limits depending on the material strength were successfully reproduced by the proposed model. The transition of the crack growth rate was also accurately predicted compared with the experimental results.
The results demonstrate that the fatigue life of steels under high-cycle fatigue can be accurately predicted from crack growth life alone. Furthermore, the proposed strategy is capable of effectively explaining the dependence of fatigue strength on microstructure and loading conditions based on the advanced fracture mechanics.

Recent advances in meshfree and particle methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATION OF THE 2D AND 3D COUPLED MULTI-RESOLUTION PARTICLE METHOD TO WATER WAVE PROBLEMS IN COASTAL ENGINEERING

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ABSTRACT

This study enhances the boundary conditions of a multiresolution particle method that combines two-dimensional and three-dimensional subdomains [1]. The multiresolution method is based on the moving particle semi-implicit method and the overlapping particle technique for multiresolution simulation of particle methods [2]. The objective is to compute fluid phenomena related to water waves in coastal engineering with reduced computational cost while maintaining accuracy. Using these improvements, water waves mimicking a tsunami on a structure are simulated and the pressure acting on the structure is compared with experimental data.

In addition, a model of wave-dissipating blocks is developed to prevent the collapse of the blocks due to water waves and to elucidate the complex mechanisms involved. The wave-dissipating blocks are treated as rigid bodies using the energy-tracking impulse method for multiple-body contacts [3]. Coulomb friction is considered to account for the frictional force acting on the wave-dissipating blocks. Using this model together with the proposed multi-resolution particle method, the interaction between the wave-dissipating blocks and the water waves is computed, and the simulation results are compared with the experiment.

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Advanced materials and smart structures: Modeling, simulation and testing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMAGE-BASED FEEDBACK CONTROL OF TEMPORARY PEDESTRIAN BRIDGES USING NEUTRAL EQUILIBRIUM MECHANISMS

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ABSTRACT

As walking and cycling paths become more densely populated, the development of infrastructure is crucial to support the transition to these sustainable transportation options. However, various obstacles such as heavy traffic roads and rivers can hinder the movement of cyclists and pedestrians. This research aims to address urban traffic challenges by creating an innovative obstacle crossing technology that is cost-effective, easy to set up, and agile.

The design of pedestrian bridges is frequently limited by deformation, and it is crucial to uphold the bridge's lightweight properties while ensuring safety and comfort. The neutral equilibrium mechanism (NEM)[1] is a zero-power control mechanism capable of managing substantial forces with exceptionally low energy demands. This active control system adjusts the reactive force at specific locations of the bridge structure to compensate the deflection displacement of those points. The control system thus behaves as a "virtual pier".

In a closed-loop control system, stable feedback signals are crucial to the efficiency and stability of the control system. This study uses digital image correlation (DIC) technology to measure the deformation of the bridge, the measured displacements are thus used as input of the control system. These actions must be performed online, and the process of measuring the state and adjusting the reaction force needs to be completed in a very short time.

Since DIC is a computationally intensive image pairing technology, in order to achieve high-frequency measurements, we used CPU multi-thread parallel processing to complete the image pairing and the computational work of control commands.

In order to verify the control efficiency and stability of the NEM-based virtual pier, a series of experiments were conducted. Experimental results show that using DIC to measure bridge status signals can reflect the advantages of high sampling rate and low noise-signal ratio. Therefore, a higher control gain can be used to improve the deformation control effect while maintaining system stability. The test results of changing the load value and load movement speed show that the control technology proposed in this article can reduce the bridge mid-span deflection displacement by 97%, achieving the control goal of the virtual bridge pier. Repeated system stability experiments have also proven high system reliability. The proposed control system indeed improved the performance of the temporary pedestrian bridge.

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Machine learning algorithms for accelerating material characterization, discovery, design, and manufacturing processes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FEATURE DISCOVERY USING MULTIMODAL AUTOENCODERS

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ABSTRACT

Materials are often characterized by a variety of modalities, e.g., process parameters, material properties, microstructure, chemistries, and performance. Parsing this onslaught of disparate data is a time-consuming process traditionally tasked to subject matter experts. However, representation learning algorithms provide a potential alternative way to make sense of these multimodal datasets. We present physics-informed multimodal autoencoders (PIMA): a variational inference framework for discovering shared information in multimodal materials datasets. In this presentation we demonstrate various capabilities of PIMA, including training on datasets with missing modalities, constructing disentangled, interpretable latent spaces, performing informative cross-modal inference, and generating new experimental process conditions which suggest desirable material properties.

Imaging-based methods in computational medicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BRAIN TISSUE SOFTENING AFTER REPETITIVE HEAD IMPACT OBSERVED FROM SUBJECT-SPECIFIC FE MODELS GENERATED WITH DIFFUSION TENSOR MRI

Vickie Shim[12], Tayebi Maryam[2], Eryn Kwon[21], Justin Fernandez[1] and Samantha Holdsworth[21]*

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[2]*Matai Medical Research Institute*

ABSTRACT

How do repetitive head impacts affect the developing brain? Participation in sports activities has sensorimotor and cognitive benefits, particularly in adolescents. However, such benefits come with the risk of brain injuries for collision sports. Some researchers suggested that the plasticity of the young brain increases the impact tolerance and recovery. Still, others suggested the opposite - that developing brains are more vulnerable than adults due to the immaturity of their nervous system. Our study aims to investigate the microstructural and tissue level changes in the brains of high school rugby players with subject-specific FE models generated with the players' diffusion tensor MR images.
We studied male high school rugby players (n=30) in Gisborne, New Zealand, for the past two years. The subjects were grouped into – 1) repetitive head impact (RHI) who did not experience brain concussion but still received sub-concussive head impacts during games and practices; 2) mTBI cohort who were clinically diagnosed with brain concussion; 3) age and ethnicity matched control cohort. The MRI scans were taken at three-time points – early, mid & post-season - to measure changes in the brain over the whole season. Players were also given a bespoke instrumented mouthguard (hitIQ, Australia) moulded to fit their oral cavity to measure the linear and angular acceleration of participant's head impacts. Players wore their mouthguards at all games and practices, allowing us to monitor the head impact frequencies and severity throughout the season.

We then used our validated semi-automated subject-specific finite element (FE) model generation pipeline [1,2]. We developed subject-specific brain FE models using their pre-, mid and post-season MRI to capture their geometry and material properties. A total of 90 subject-specific FE models were developed. These fully subject-specific model generated subjects' unique strain patterns when run with their impact profiles measured with instrumented mouthguard sensors. In particular, we observed brain tissue changes in those players after one season. When simulated with the same head impact, the brain models generated with post-season MRI scans showed much higher strain than the one developed with preseason MRI. This may mean brain tissue has become softer due to small but repetitive head impacts from games and practices. This finding and its potential biophysical meanings from multimodal MRI scans will be presented at the meeting.

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Numerical modelling of composite materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TWO-SCALE DAMAGE PROPAGATION/STRENGTH ANALYSIS OF CFRP CONSIDERING RANDOMNESS OF FIBER DISTRIBUTION

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ABSTRACT

Carbon fiber-reinforced plastics (CFRP) are used as structural materials in aerospace and energy applications, because of their higher specific strength, specific stiffness, and corrosion resistance compared to common metal materials. In general, CFRP are manufactured by stacking laminae (plies) which are submillimeter thick resin sheets unidirectionally reinforced by a number of carbon fibers with diameters of 5-10 micrometers. Thus, when CFRP are subjected to relatively large load, micro-scale damages such as resin cracking, fiber/resin interface debonding and fiber fracture firstly occur in laminae, and then they progress and accumulate, leading to macro-scale stiffness degradation and failure. Therefore, analyses considering microscopic damage behavior are required to predict damage/strength properties of CFRP.

For the above reason, this research group has developed a two-scale damage analysis method by introducing damage criteria into a two-scale analysis method based on a homogenization theory [1], which can explicitly couple microscopic damage propagation and macroscopic strength of CFRP. In this study, however, the randomness of fiber distribution observed in actual CFRP was not considered, and thus it did not accurately capture actual damage behavior of CFRP.

In this study, two-scale damage/strength analysis of CFRP that takes into account the randomness of fiber distribution is performed. For this, several unit cell models with random fiber distribution [2] are prepared as microscopic models of laminae. Then, they are randomly assigned at integration points in a macroscopic model of CFRP, and the two-scale tensile analysis of CFRP is performed. In the analysis, CFRP with several different laminate configurations are considered, and the effects of random fiber distribution on the damage and strength properties of the CFRP are investigated by comparing the results with and without considering the randomness of fiber distribution.

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Innovations in machine learning-enhanced uncertainty quantification for computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPANSION OF DEEP MATERIAL NETWORK FOR WOVEN COMPOSITE THERMAL CONDUCTIVITY HOMOGENIZATION

Dongil Shin[*1], Peter Creveling[1], Scott Roberts[1] and Remi Dingreville[1]*

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ABSTRACT

Developing reduced-order models to accelerate simulations has garnered significant attention across diverse physics domains. Artificial intelligence has contributed significantly to this aspect of computational speed improvement in the last decades. One of the primary interests is micro- and mesoscale surrogate models for multiscale interpretation. Deep Material Network (DMN) represents a novel approach that goes beyond predicting homogeneous properties directly through physics-informed machine learning models. During the last few years, it has generated substantial interest in the mechanics of microstructures. However, existing DMN research has predominantly focused on network parameters related to mechanical behavior. This study seeks to extend DMN research to address thermal conductivity homogenization in woven structures. Through an in-depth study of DMN models, this research aims to concretize network and node parameters, providing a comprehensive framework for extending the DMN to other physics domains. To account for anisotropy, particularly relevant in the case of woven structures, we explore how expanding network parameters can enhance prediction accuracy, building upon existing research approaches. Our interpretation results showcase the ability to predict homogeneous and thermal conductivity properties over a thousand times faster, facilitating uncertainty quantification (UQ) studies and sensitivity analyses in coupled scale scenarios. This research contributes to the understanding that DMN is not limited to elastic problems but can be effectively applied to other physics when properly defining relationships between constitutive equations and network parameters. By demonstrating the potential for extending DMN to other physics domains and modeling degrees of freedom, this study lays the groundwork for solving multi-physics problems via DMN. Sandia National Laboratories is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

Advances in damage & fracture modeling of multiphysics materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ANALYSIS OF THE DAMAGE BY THERMAL LOADING IN A HETEROGENEOUS INTEGRATION PACKAGE

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ABSTRACT

A heterojunction package is one in which various types of individually manufactured chips are assembled and integrated to a level comparable to the size of a single chip. It integrates chips with various functions such as processor, memory, sensor, optical, and MEMS, and is electrically connected using rewiring, micro bumps, copper direct bonding, and through silicon via. Because the heterogeneous packages are manufactured considering complex factors such as various sizes, materials, process conditions, and manufacturing technology, it is considered important to secure mechanical reliability.

As the structure of the package becomes more complicated and the number of materials increases, it is vulnerable to damage depending on the manufacturing process and user usage environment. This has led to changes in both the microstructure and mechanical properties of interfaces and joints in the package. The creep behavior of solder joints is particularly important to predict due to the complex time-temperature dependence of solder behavior.

In this study, a numerical analysis was performed in order to evaluate the damage in the heterogeneous integration package. The structures of the packages were designed and corresponding manufacturing processes were considered. The constitutive models for material properties were developed. Damage response was used to gauge the rate of degradation and predict the life of the joints. Numerical results were verified by the measurement of thermal deformation.

Deep and machine learning methodology in the context of application to computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ACOUSTIC BARRIER DESIGN WITH TOPOLOGY OPTIMIZATION BASED ON DEEP REINFORCEMENT LEARNING

Myung Shin[1] and Gil Ho Yoon*[1]

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ABSTRACT

This research employs a topology optimization based on deep reinforcement learning technique to design sound barriers for noise reduction. Reinforcement learning is a type of machine learning in which an agent gradually learns to find the optimized solution through various experiences in a situation where there is no data. Reinforcement learning can be applied by decomposing the topology optimization process into iteratively adding elements. In this study, we delve into the topology optimization of acoustic systems using Double Deep Q-Network (DDQN), a famous algorithm in deep reinforcement learning. The agent in reinforcement learning observes the acoustic fields, boundary conditions, noise source positions, and the location of the target area. The RL agent takes actions to add solid materials starting from an empty design space. The reward is defined as the difference in the objective function before and after material addition. The goal of the reinforcement learning agent is to find a solid element addition policy that achieves the maximum cumulative reward, which ultimately finds the topology of the barrier structure that minimizes the sum of the absolute values of sound pressure in the target area at multiple frequencies. Through numerical examples of sound barrier design, this study validates the reliability of the reinforcement learning-based acoustic topology optimization technique. The results demonstrate that the reinforcement learning agent effectively performs multi-frequencies acoustic topology optimization in various boundary conditions, locations of noise source and objective areas.

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Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A CDM-LIKE CONSTITUTIVE LAW COMBINED WITH TRESCA YIELD FUNCTION TO PREDICT SHEAR-LIP FRACTURE ALONG WITH STRAIN LOCALIZATION

Yuichi Shintaku[*1], Reiya Tao[1] and Kenjiro Terada[2]*

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ABSTRACT

We present a continuum-damage-model-like constitutive law embeding cohesive cracks with Tresca yield function to predict shear-lip fracture along with localization. The proposed constitutive law accommodates a hyper-elasticity based plastic model with the use of the deformation gradient multiplicatively decomposed into separation-induced, elastic and plastic parts. The elastic–plastic deformation along with isotropic hardening is represented by a Hencky-type model combined with the Tresca yield function. In addition, the strain softening due to the shear-lip fractur along with the strain localization is represented by the introduction of the shear-induced damage variable into the Tresca yield function. The evolution of the shear-induced damage variable is represented by the damage-loading function corresponding to the plastic energy release based on thermodynamics. On the other hand, the stress release process caused by flat fracture is realized by cohesive traction separation law and the assumption of the local equilibrium state between the principal stress and cohesive traction. By comparing with results of a CDM-like constitutive law combined with Mises yield function, the capability of our proposed model is demonstrated throughout the various types of specimens under different stress states.

Machine learning for design tasks and inverse problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTITASK REPRESENTATION LEARNING FOR STRUCTURAL DESIGN

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ABSTRACT

In product development, it is necessary to design structures that satisfy multiple constraint conditions. In the early stages of product development, where the actual product is not available, evaluation using CAE is employed. By incorporating CAE results and updating the shape accordingly, it is possible to design an optimized shape that meets the objectives. However, if the need for shape changes arises during the product development process, it requires a reevaluation involving the aforementioned shape design and CAE evaluation.

In this study, we propose a Neural Network model, that simultaneously achieves the tasks of automatic shape generation and inference of CAE evaluation results. With the proposed model, it is possible to generate a modified shape, predict the distribution of corresponding physical quantities, and estimate the cost function in real-time. This capability contributes to smoothing the designer's workflow and enhancing the efficiency of the development process.

The proposed model utilizes a shape representation based on point clouds, consisting of an encoder that extracts the latent vector of object shape from the point cloud and a decoder that reconstructs the point cloud from the latent vector. Additionally, the model includes regression models to determine the physical quantities at each point of the point cloud from the latent vector and to calculate the cost function value.

In the algorithm for shape generation, this study proposes intentionally adding points sampled on the boundary of the shape, in addition to uniformly sampling points on the conventional shape surface during point cloud creation. The intentional inclusion of boundary points through focused sampling is expected to improve the reproducibility of shapes and enhance the prediction accuracy of CAE results on the boundary.

To verify the effectiveness of the proposed method, a practical numerical example is demonstrated.

Fluid-structure interaction in interface and moving boundary problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HIERARCHICAL REDUCED ORDER MODELING FOR DISTRIBUTED MEMORY PARALLEL COMPUTERS

Kyohei Shintate[*1], Naoki Morita[1], Shigeki Kaneko[2] and Naoto Mitsume[1]*

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ABSTRACT

Model order reduction techniques represent a very effective approach for computationally intensive applications involving the repeated solution of parametric Partial Differential Equations (PDEs), which arise from various fields such as optimal control, shape optimization, fluid dynamics, and structural dynamics. On the other hand, the efficiency of these systems is constrained by the curse of parameter dimensionality due to the complexities of PDEs and high computational costs in the offline stage. To tackle these issues, the combination of Reduced Order Models (ROMs) and Domain Decomposition Methods (DDM) has been explored to reduce the parameters and degrees of freedom in parametric PDEs. The common idea behind these methods is to construct local reduced spaces on each decomposed subdomain and combine these spaces across interfaces. Although various coupling methods such as iterative Schwarz method or Lagrange multiplier method exist, there are few examples implemented in distributed memory parallel computers, which are highly valuable for memory usage. Additionally, there is a lack of discussion on parallel computational performance, a critical aspect in DDM.

In this study, aiming to fundamentally address memory usage and computational bottlenecks, we propose an overlapping DDM for distributed memory computers, based on generalized hierarchical graph decomposition. Hierarchical graphs consist of a three-level architecture corresponding to mesh nodes, ROM computation subdomains, and parallel computation subdomains, respectively, which are associated using DDM. The proposed method employs Local Proper Orthogonal Decomposition (LPOD)[1] as the basis selection method for ROM computation subdomains, allowing the independent determination of bases for each one. Since it interacts only with neighboring subdomains, the POD computation subdomain is considered a graph node. The hierarchical graph structure of our proposed method allows independent definitions of POD computation subdomains and parallel computation subdomains. By representing these relationships as a graph, we successfully enable parallel computation in distributed memory computers. We discuss the computing efficiency and parallel computational performance through its application in fluid analysis.

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Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE PHASE FIELD APPROACH FOR MIXED-MODE FRACTURE MODELLING TO UNDERSTAND INSTABILITY IN THE MATERIALS

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ABSTRACT

The instability is the unexpected deviation in crack growth process. The deviation in the crack growth is seen due to the stress state of the crack front. The crack kinking is the effect of the stress state parallel to the crack front. This stress is responsible for the instability of the crack path. In the case of the materials with interfaces, crack propagation is seen in the events of penetration and deflection (Hutchinson, 1989) . The competition of penetration of the crack inside the material and deflection of the crack along the interface depend on the fracture toughness of the interface and material. As the crack progresses, the energy release rate increases more than the critical fracture toughness of the material. The excess energy is responsible for the crack to meander in the form of oscillations. Sometimes, the crack tip of the accelerating crack becomes blunt and splits into the branches, creating a crack-branching event. These events are seen in brittle materials like glasses.

The study aims to understand the point of instability in the crack propagation process. The phase-field framework can be used to model the instability in crack propagation. The stress-based failure criterion can be used to track the nucleation and evolution of the crack growth process (T. Clayton, 2022). The anisotropic nature of the material can be given in the total energy equation of the system (Shariff, 2022). This equation can then be used for solving the evolution of the crack.

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Recent advances in meshfree and particle methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMPROVED DENSITY-BASED PARTICLE SHIFTING TECHNIQUE FOR STABLE AND ACCURATE FREE SURFACE FLOW SIMULATIONS BASED ON SPH(2)

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ABSTRACT

In recent years, along with climate change related to global warming, natural disasters have become more frequent and severe, and numerical simulations are required to accurately predict disaster damage of unknown scale that may occur in the future. The particle method is suitable for tsunamis, flooding, and sediment disasters because it is good at representing intense deformation such as splitting and merging, but it is prone to accuracy degradation and numerical instability due to disorder in the particle placement. To solve these problems, SPH(2) has been proposed, which enables highly accurate operation even in the particle placement disorder. The SPH(2) gives a better accuracy and convergence property compared to traditional SPHs, but it still has a limitation to overcome the numerical instability. Particle Shifting Techniques has been proposed to keep a better particle homogeneous particle placement, but long-term volume conservation has not been discussed carefully. On the other hands, a stabilized ISPH[1], in which an artificial source term to satisfy the density invariance in the pressure Poisson equation is introduced, can control the total volume.In this study, we propose a new Particle Shifting without the artificial source term of the pressure Poisson equation. This is a simple combination of the existing Optimized Particle Shifting (OPS) [2] and the Density-based PS[3] to simultaneously improve particle placement and volume conservation. Finally, the numerical stability and accuracy improvement of the proposed method are demonstrated by rotating square patch of fluid and dam break simulations.

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Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE MODELING OF MICROSTRUCTURED BEAMS BASED ON MICROMORPHIC THEORY

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ABSTRACT

Metamaterials are artificial materials with novel properties and functionalities not found in natural materials. They have potential applications in various fields, including acoustics, optics, mechanics, and thermodynamics. However, analyzing metamaterials is challenging due to the complex interactions between the macro and micro scales [1]. Here, we investigate an efficient multiscale model for metamaterial beams' linear and nonlinear bending and vibration behavior.
A micromorphic beam theory is developed from the conventional Timoshenko beam theory using independent axial and shear strains and rotations at the microscale level [2]. This enables an accurate description of the deformation of the microstructured beams with only a few unit cells through the thickness direction. The micromorphic Timoshenko beam captures size effects and is more computationally efficient than 2D or 3D micromorphic continuum models.
One of the main aspects of this research is to identify micromorphic material parameters by comparing them with representative volume elements of the microstructure. This is done by using a differential quadrature method to numerically discretize the governing equations for static deformations as well as vibrations. The numerical examples demonstrate the accuracy of the method in obtaining deflections, linear eigenfrequencies, and nonlinear frequency responses for metamaterial beams with weakly separated macro- and microscales.
Our work is a contribution to the field of the theory of micromorphic beams and the multiscale modeling of metamaterials. The proposed approach is efficient and accurate in capturing the nonlinear beam behavior. A systematic procedure for identifying micromorphic material parameters from the microstructure is also provided.

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SciML in the real world
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BAYESIAN NEURAL NETWORK PDE SOLVERS WITH UNCERTAINTY QUANTIFICATION AND GENERALIZABILITY ACROSS BVPS

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ABSTRACT

Solving Partial Differential Equations (PDEs) is essential for understanding the behavior of physical systems. However, large-scale solutions of PDEs, even with state-of-the-art discretization techniques, remain costly. We propose a novel physics-constrained neural network (NN) approach for solving PDEs without labels, facilitating high-throughput solutions for design and decision-making. Unlike traditional physics-informed NN approaches that rely on the strong or weak form of PDEs for the loss function, our method constructs the NN's loss function using the discretized residual of PDEs, implemented efficiently through a convolutional, operator-based, and vectorized approach. In addition to a deterministic model, we develop a probabilistic model by incorporating Bayesian NNs (BNNs) to quantify the epistemic uncertainty from model parameters and aleatoric uncertainty from data noise. For BNNs, the discretized residual forms the basis of the likelihood function. Our approach utilizes deterministic and probabilistic convolutional layers to learn the applied boundary conditions (BCs) and identify the problem domain. With Dirichlet and Neumann BCs as inputs, a single NN can address similar physics across various BCs and problem domains. The trained surrogate PDE solvers can interpolate and extrapolate predictions for BCs beyond their training exposure. This is particularly useful for problems requiring repetitive solutions of similar PDEs with minor variations. We demonstrate the effectiveness and performance of our framework on a range of steady-state and equilibrium boundary value problems, encompassing diffusion, linear elasticity, and nonlinear elasticity.

Machine learning for design tasks and inverse problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

OPTIMIZING FIBRILLAR ADHESION DESIGN USING SUPERVISED MACHINE LEARNING

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ABSTRACT

Fibrillar adhesion is a natural phenomenon found in many living organisms, including flies, spiders, and geckos. This adhesion mechanism relies on small hair-like structures, called fibrils, attached to a backing layer which enhances adhesion to surfaces, allowing these organisms to climb vertical surfaces. Inspired by this mechanism, there are many applications that utilize fibrillar adhesion to increase their adhesion performance, including in robotics and medical devices. The stiffness of the fibrils and backing layer, along with the length, distance, and configuration shape of the fibrils, are critical structural parameters that determine the maximum adhesive strength of the fibril array [1]. However, optimizing the structural design of fibrillar adhesives to enhance their adhesive strength is a challenging task, due to the large computational cost of current numerical models. In this study, various supervised machine learning (ML) models, including linear and non-linear regressions, as well as neural networks, including ANN, DNN, and CNN, were trained to generate a reliable and fast approximation of the maximal adhesive force of a given fibrillar adhesive. The results show that deep neural networks perform best, yielding up to 10 times improved mean absolute test error compared to the baseline. The faster model provides accurate results when predicting different sizes of fibrils, different distances between fibrils, and diverse geometrical shapes of the arrays. In the next step, I designed a framework containing two DNNs with same structure and hyperparameters to optimize the fibril length distribution, for any arbitrary shape of the backing layer with fibrillar array on top to find the highest possible adhesion force in the structure. The first DNN is to be trained on training set and hyperparameter tuning and the second DNN is designed to solve the inverse problem to find the optimum solution by cutting down computation time from minutes/hours to seconds [2]. Overall, the study highlights the potential of using machine learning techniques to optimize the design of fibrillar adhesives, which could have important implications for the development of new and improved adhesives in various fields, such as robotics, medical devices, and space exploration.

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16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Minisymposium in honor of Prof. Yannis Kallinderis's 60th birthday: Progress of Unstructured grid based CFD, hybrid mesh generation and adaptation, and parallel supercomputing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PARALLELIZATION OF THE FINITE ELEMENT-BASED MESH WARPING ALGORITHM USING HYBRID PARALLEL PROGRAMMING

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ABSTRACT

Parallel dynamic meshes are essential for computational simulations of large-scale scientific and engineering applications involving motion, such as the launch of a rocket into outer space, the swaying of a building due to an earthquake, and the beating of a human heart. Although there are several parallel implementations of mesh warping algorithms in existence, all of them have been developed for enhanced scalability exclusively for shared or distributed architectures. None of them have been designed to take advantage of MPI-3's shared memory programming, an all-MPI alternative to MPI/OpenMP programming. For example, they do not consider the remote memory access (RMA) or shared memory (SHM) communication features available in MPI-3. Considering that the core count in compute nodes, from laptops to high-end servers, continues to increase, we hypothesize that utilizing MPI RMA and SHM features will provide a superior solution, in terms of scalability, over existing approaches to parallel mesh warping algorithms that utilize exclusively shared or distributed memory programming.

In this talk, we discuss our parallelization of the finite element-based mesh warping (FEMWARP) algorithm, which was proposed by Shontz and Vavasis. Our parallel implementation takes advantage of the features of MPI RMA and SHM communication to solve a Poisson boundary value problem for the deformed mesh. The first step of the FEMWARP algorithm is to compute a set of local weights for each interior node which describe the relative distances of the node to each of its neighbors. This involves generating a global stiffness matrix and solving for the sets of weights in an embarrassingly parallel manner. To assist in the computation, the neighbor lists for each interior node are pre-computed using hybrid parallelism. The second step of the FEMWARP algorithm is to apply the boundary transformation from the application in an embarrassingly parallel manner. Finally, new coordinates for the interior nodes are computed by solving a system of linear equations with multiple right-hand sides that is based on the weights and boundary deformation. A Preconditioned Block Conjugate Gradient Method is used to solve equations. Our numerical results demonstrate good efficiency and strong scalability of parallel FEMWARP on up to 256 cores on the KU Community Cluster.

Analytical models for nonlinear dynamics and evolved dynamics in natural, social and engineering sciences
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMPACT CRATERS OF THE MOON WITHOUT SIGNS OF THE MATTER MELTING AND THE MATTER EMISSIONS

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ABSTRACT

The classic idea of impact craters is that all craters are divided into two groups: simple and complex. However, the achievements of orbital observations in recent years have made it possible to detect craters that do not belong to these two groups.
The authors examined the area of "bulbous fields" at the bottom of the young Aitken crater to understand the unusual topography of a group of 5 small craters included in the named area. During the analysis, one of the five craters attracted attention by the topography of the bottom. There was no melt of matter in the form of solidified magma at its bottom, as happens in simple craters. But there are no also central peak there! Instead, a smooth convex surface covered with small impact craters is confidently visible. It is also characteristic that in the vicinity of this crater there is no material of the substance ejected as a result of the impact that led to the formation of the crater. As a working hypothesis, the authors suggested that the described crater contains the body of the impactor, which deepened when falling into the molten lake of the Aitken crater bottom.
At the same time, the impactor did not undergo destruction. This could be due to the fact that at the time of the shock of the drummer, the surface of the Aitken bottom had not yet completely cooled down, and the melt substance was in a viscous state. As a result of the introduction of the impactor's body into the Aitken bottom, a shock wave arose, which led to the formation of domes of "bulbous fields". The energy of this shock wave was apparently enough not only to form domes, but also to penetrate the coating of the Aitken bottom in two places near the edges of craters with domes and create lava tubes, which are clearly visible in ultra-high resolution images.
Our report attempts to find similar craters in other regions of the Moon. The presence of such craters on the Moon is not only of theoretical interest, since it expands and complements the generally accepted idea of simple and complex craters. The practical significance of such craters lies in the fact that small asteroids, meteorites or fragments of them may turn out to be preserved impactors.
Then such craters appear to be objects of increased interest for upcoming lunar expeditions

Machine learning algorithms for accelerating material characterization, discovery, design, and manufacturing processes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LEARNING PROCESS-STRUCTURAL-PROPERTY RELATIONS IN MICROSTRUCTURES THROUGH MULTI-MODAL BASED MACHINE LEARNING.

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ABSTRACT

This presentation will discuss a multi-modal-based machine learning approach for building the process-structural-property relations for the Molybdenum (Mo) thin films fabricated using various physical vapor deposition (PVD) processing conditions.

Material such as Mo thin films, due to their excellent physical properties, play a crucial role in the semiconductor industry. Consequently, there is a growing interest in producing these films with exceptional properties to enhance the efficiency and reliability of semiconductor devices. However, producing thin films with desired properties requires knowledge of process-property relationships. Machine learning models are highly efficient in learning complex relations between diverse processing conditions and multiple properties. To increase confidence in these machine learning models, they must be enabled to capture and disseminate knowledge that is interpretable by material science experts. This knowledge is mainly desired through PSP linkage (Process-Strcture-Property). In the existing research, the machine learning models used to study PSP correlations have been limited, likely because of the multi-modal nature of microstructural data.

In order to utilize the multi-modal information, a multi-modal-based machine learning approach was developed that predicts the properties and microstructural characteristics of the Mo thin films from the given PVD processing conditions. First, a multi-modal deep learning model is used to learn a joint latent representation of the multi-modal microstructure data. Then, another deep learning model is used to learn a relationship between the processing parameters and the joint latent representation. The predicted joint latent representation for given processing conditions can be then reconstructed into original multi-modal structural information that is interpretable by material science experts.

The Mo thin films were deposited onto Si wafers using the PVD technique for various Ar pressures and sputter powers. Here, the processing conditions, pressure, and power are input for the deep learning model that predicts a joint latent representation of the multi-modal information about the thin films. The multi-modal structural information about thin films is obtained using high-throughput experimentation. The information consists of 1D spectral data in the form of X-ray diffraction (XRD), 2D images in the form of scanning electron microscopy (SEM) and transmission electron microscopy (TEM), and scalar dataset in the form of resistivity.

MECHANISTIC STUDY OF THE DEGRADATION MECHANISM OF LITHIUM-ION BATTERIES

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ABSTRACT

Lithium-ion batteries (LiBs) are stable portable energy sources and finding increased use across the industry from consumer electronic segment to electric vehicle (1). LiBs suffer from challenges in reliability during fast charging, long repeated cycles, high temperature operation and low temperature operation. The repeated charging and discharging of the LiBs result in capacity loss due to the deposition of cyclable lithium as solid electrolyte interface (SEI) layer on the anode surface and cathode interface layer (CEI) on the cathode (2). Additionally, lithium ions are also susceptible to deposition as Li Metal on anode surface during fast charging or lower temperature charging resulting in large capacity losses. The mechanical stress associated with intercalation and deintercalation of lithium from the electrode particles may result in particle cracks. The dendrite growth due to lithium plating may impact separator integrity and increasing risks of runaway heating and catastrophic failure. Hence, understanding the capacity loss due to electrolyte interface growth and plating is essential to ensure safe operation of LiBs.

We utilize a previously reported single particle model (SPM) that incorporate battery damage mechanism of SEI growth, SEI cracking, lithium plating to estimate capacity losses and battery degradation during repeated fast charging of batteries (3). The model predictions are compared to experimental measurements of capacity losses to validate the modeling assumptions and determine the parameters required to describe the damage models. The experimentally validated SPM model is utilized to get critical insight of the behavior of the different degradation phenomena during repeated cyclic operation. The model is used to characterize irreversible plating growth with C rate, SEI film growth rate and film resistance variation rate, the loss in capacity and cell voltage characteristics with the experimental result across different spectrum of C rate 0.1C to 6C. The close agreement between the model predictions and experimental result showed model's capability to characterize the performance degradation of LiBs.

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Machine learning for design tasks and inverse problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LEVERAGING GANS AND CNN FOR STRESS MITIGATED DESIGN GENERATION

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ABSTRACT

Abstract:
Design generation and optimization using state-of-the-art deep learning (DL) methods, especially generative designs (e.g., generative adversarial networks (GANs)), have emerged as a powerful tool in engineering. However, ensuring the structural integrity of these GAN-generated designs remains a challenge to overcome. This work proposes an innovative approach that integrates a Convolutional Neural Network (CNN) based predictive model and generative adversarial network to iteratively generate designs with improved structural reliability. This work aims to employ Convolutional Neural Networks (CNNs) for predicting stress levels in designs generated by GANs and utilize these predictions to mitigate overall stress. The CNN model is trained on a dataset of stress-annotated designs, enabling the model to learn complex patterns between design features and corresponding structural stress. Once trained, the CNN becomes a stress prediction tool. When the GAN generates a design, it undergoes stress assessment through the CNN. The predicted stress value is used as a threshold to reduce the induced stress in each design. Integrating CNN-based stress prediction into the GAN workflow results in designs with lower stress levels while maintaining structural robustness and design diversity.

This research has profound implications, especially in industries requiring rapid generation of optimized designs, such as aerospace and automotive engineering. By utilizing CNNs to predict and minimize stress in GAN-generated designs, the approach enhances the efficiency and reliability of the design generation process. It ultimately improves product performance and safety. This research introduces a novel methodology for integrating CNN-based stress prediction into GAN-generated designs, showcasing its potential to revolutionize design optimization across various engineering domains.

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Modeling, simulation, and AI for ultrasonic NDT and SHM
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A SURROGATE FOR RAPID EVALUATION OF GUIDED WAVES IN PLATES WITH MULTIPLE DEFECTS

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ABSTRACT

Guided Waves form an efficient method for Structural Health Monitoring (SHM) and Non-Destructive Evaluation (NDE) of thin plate structures. This technique exploits the favorable properties describing the propagation of Lamb waves, such as low geometrical damping, which permits the coverage of extended areas with few low-cost PZT sensors, and a short wave length, which enables the detection of minor defects. The latter leads to drawbacks regarding the forward simulation of the wave propagation phenomenon, which is though an essential task when a model-based method is adopted. Model-based schemes can offer advantages over purely data-driven schemes, since they offer the potential for extrapolation and response estimation in unmeasured location. However, as short wave lengths require a fine discretization in space and time, they are linked with a high numerical toll; this poses a significant obstacle in the implementation of computationally intensive tasks, such as inverse problem solutions related to localization and quantification of defects.

A surrogate model can be deployed to expedite the task of forward simulation, which forms a necessary part of any inverse setting. Within an inverse formulation, such a surrogate needs to be parameterized concerning the characteristics of candidate defects, e.g. in terms of the defect positioning and size, in order to ensure rapid evaluations. This contribution presents a surrogate model, which couples ray tracing of Lamb waves with Frequency Response Functions (FRFs) to get the response at various sensor locations. The method enables the simulation of multiple defects and features within plate geometries, such as rivet holes. The efficiency of the surrogate in an inverse setting is demonstrated in a synthetic, numerical example with conical notches and conical holes as defects.

Modeling and simulation of dynamics, stability and control of aerospace structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STUDY OF THE DYNAMIC BEHAVIOR OF CELLULAR STRUCTURES FOR THE ABSORPTION OF MECHANICAL VIBRATIONS

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ABSTRACT

In the structural engineering, vibration can be a problem that can cause serious problems and even endanger human life if not properly considered in the design phase. Several active and passive mechanisms have been developed over time to damp its effects, however, most of them have some drawbacks, such as low static stiffness, complex design, attenuation in a limited frequency and more. As additive manufacturing was developed, cellular structures became possible to be manufactured in a single piece. In order, to overcome limitations of current attenuating mechanisms, the use of local resonators within the cellular structure had been proposed to combine the advantages of repetitive structure with the advantages of the resonators through the elastic band gap effect. Therefore, the focus of this work was to evaluate the dynamic behavior of 2D cellular structures using the finite element method, with local resonators calibrated to damp vibrations at a specific excitation frequency, to understand their advantages and capabilities. Even though some unexpected effects of signal amplification may happen in frequencies not originally considered, attenuation of specific excitation frequencies in a simple way by using local resonators associated with cellular structures was observed.

16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics

July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODEL COMBINATIONS USING FUZZY CONTROL

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ABSTRACT

Combining forecasts from multiple models is a commonly used method to achieve more accurate results than relying on a single model. This approach is widely adopted in fields such as meteorology, hydrology, and economics. It is established that using model combinations in practical applications typically leads to better performance compared to using a single selected method. However, the real advantage of combining models lies in their ability to mitigate risk, offering a more reliable outcome than the selection among individual models.

In our work, we use models that consider uncertainties represented by fuzzy numbers, so our Quantity of Interest is also represented by fuzzy numbers. Our primary focus is to explore how to combine these fuzzy numbers. There are various techniques available to combine them. However, all of these techniques assume that all fuzzy numbers have equal reliability. In some cases, this assumption can be incorrect, posing a potential risk in the combination process. To avoid risks, we will use a compatibility function to determine whether all information can be fused or whether it is too conflicted to make an adequate combination.

To address the inherent subjectivity and uncertainty inherent in assessing information reliability, we employ fuzzy control, a widely recognized method for managing systems characterized by imprecise components.

In our work, the decision on what and how to combine is made by a fuzzy control. This control selects which models to combine based on a conflict measure. Additionally, the control determines the fusion strategy to be employed.

We illustrate the implementation of this control in tackling the heat exchanger fouling problem, a problem that has multiple sources of uncertainties that can profoundly affect the efficiency and performance of various industrial processes.

New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION APPLIED TO 3D COMPRESSIBLE SUBSONIC ROTOR DESIGN USING FINITE DIFFERENCE ADJOINT APPROACH

Felipe Silva Maffei[*1], Carlos Massaiti Okubo Junior[1], Julio Romano Meneghini[1] and Emílio Carlos Nelli Silva[1]*

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ABSTRACT

One of the main challenges of topology optimization for turbulent compressible flow problems is to have an efficient way to calculate the sensitivities in such flow conditions. The present paper extends the work of Okubo et al. [1] (compressible laminar flow) by incorporating turbulence in the sensitivity calculation (via the discrete adjoint method), making it possible to evaluate the sensitivities considering this phenomenon. The methodology can be summarized as follows. The forward problem is solved using the finite volume method. Using the discrete set of governing equations, the adjoint system is mounted (with the terms of the derivatives being approximated by finite differences) and solved. With the adjoint field and the gradient of residual w.r.t design variable, the sensitivity is evaluated. Then the design variables are updated, and the loop continues until the termination criteria are achieved. In this work, the forward problem takes advantage of the already implemented parallel computing of OpenFOAM. The MMA solver is used to update the design variables. The methodology is applied to 3D rotors, i.e. a practical example of compressible turbulent flows. Two objective functions are used: the minimization of entropy flux and the minimization of total pressure flux.

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Contact and interface mechanics: Modeling and computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL AND PHYSICAL ASPECTS ON ADHESIVE AND FRICTIONAL INTERACTION FOR ROUGH CONTACT SIMULATION

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ABSTRACT

Understanding the interplay of adhesion and friction in the contact of rough surfaces is still an open challenge within the tribology community. Specialised computational tools designed towards this purpose are becoming more valuable in building accurate and robust simulations of adhesive effects in complex multi-physical and multi-scale systems. Particularly, the development of numerical models at finite strain incorporating roughness, adhesion and friction is still an actively researched problem [1].

In our approach, we propose an implementation of the Raous, Cangemi, and Cocus (RCC) model [2] under the finite deformation dual-mortar contact framework. By combining Frémond's adhesion intensity concept, which models adhesion through a damage-like state variable, with strict inequalities for unilateral contact and Coulomb friction conditions, this model seamlessly combines adhesion with sliding friction. To enforce the RCC constraints a nodal lumping technique is used and a primal-dual active set strategy is derived by introducing two novel modifications to the non-linear complementary functions.

This research explores the numerical and physical performance of the RCC model for roughness simulations. The study investigates the effect of different mortar-based kinematic variables used for the treatment of the adhesive components for a sound space discretisation. In addition, it explores the mechanism of adhesion reconstruction and bond formation to obtain stable solutions and accurate physical trends. Numerical stabilization procedures based on viscosity and inertial effects are also employed. Finally, the validity of the developed framework is assessed by comparing numerical and mechanical responses against other well-established models in the literature.

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Advanced analysis of steel and steel-concrete composite structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL FORMULATION FOR ADVANCED ANALYSIS OF SEMI-RIGID STEEL-CONCRETE COMPOSITE FRAMES

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ABSTRACT

The present work aims at the implementation and validation of a displacement-based two-dimensional numerical formulation including several sources of non-linearities in steel-concrete composite frames, such as second-order effects, plasticity and beam-to-column semi-rigid connections. The co-rotational-based approach is used to describe the finite element formulation, allowing large displacements and rotations in the numerical model. Two rotational pseudo-springs in series are positioned in the finite elements ends (Chan and Chui, 2000). One of them is used to include the gradual loss of stiffness determined by the cross-sectional plastification. The limiting of the uncracked, elastic and plastic regimes is defined in the Normal Force-Bending Moment diagram. In the cross-sectional analysis, the Strain Compatibility Method (SCM) is used to capture the axial strains in the section components. In this way, the constitutive models of the materials are described by continuous functions. The cracked effect is considered by the effective moment of inertia of the concrete cross-section (Branson and Metz, 1963). The other spring includes the effects of the semi-rigid beam-to-column connections through the moment-rotation relationship. A multi-linear model for beam-to-column connections is used. To validate the proposed numerical formulation, the results obtained are compared with numerical and experimental data available in the literature. Since the model proposed here starts with the concentrated simulation of nonlinear effects, an examination of the finite element mesh refinement is also carried out. These comparisons indicated for the validation of the numerical procedure proposed and implemented here, highlighting the precision of the formulation in both the pre- and post-critical structures behavior.
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Continuum biomechanics of active systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COUPLED ANALYSIS OF ACTIVE BIOLOGICAL PROCESSES FOR MENISCUS TISSUE REGENERATION

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ABSTRACT

This presentation is concerned with modeling, simulation and experimental validation for the meniscus regeneration and involved cell and tissue-level phenomena. The motivation for this work stems from clinical studies indicating that partial and total meniscectomies lead to prevalence of premature osteoarthritis in knee joints. Accordingly, substantial efforts are being made towards finding adequate regenerative tissue for meniscus replacement. Most regenerative approaches are clinically motivated and focus rather on the practical application than on the micro- and macroscopic cellular mechanisms and the interactions with the scaffold material. Our work is innovative in the sense that it aims to understand the basic control mechanisms in cell-scaffold interactions under different environmental parameters, thus providing a selective prognosis of the most significant combinations of these parameters. With respect to the in-silico modeling and simulation, a major challenge lies in the well-posed and numerically efficient coupling of the processes at the cell level with the macroscopic behavior and the mechanical properties of the tissue. The active processes at the cell level, such as cell differentiation and matrix synthesis, have a strong impact on the resulting tissue structure and quality, while macroscopic effects in turn are important stimuli for the processes at the microscopic level. Moreover, the time scales of the different processes differ vastly and call for appropriate co-simulation strategies. The presentation will first give an overview of the mathematical model that we have established so far and that forms a coupled system of time-dependent partial differential equations where cell densities play a dominant role. The main focus will then be placed on the numerical challenges, along with a report on the computational results that we have obtained so far and their validation with respect to experimental data. Also, recent results on non-intrusive model order reduction methods will be introduced. These turn out to be essential when tackling the parameter identification problem along with the computation of parameter sensitivities.

Data-driven approaches for solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN OPERATORS FOR ELASTIC AND ELASTIC-PLASTIC SOLIDS

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ABSTRACT

The governing equations of continua can be discretized into a system of ordinary differential equations when discretized in time. The system describes evolution of state variables such as displacements and temperatures, and their evolution can be described by operators. We show how to construct such operators for solid mechanics using displacement vector data, and for thermal systems using temperature data. The operators can reconstruct the fields as a function of space and time. No knowledge of the material properties (thermal conductivity, elastic moduli), boundary conditions, or solution of the conservation equations is required.
For linear-elastic solids, the Dynamic Mode Decomposition [1] algorithm is used. Field data is acquired as snapshots and arrayed as vectors. Time-shifted data matrices whose columns are the snapshots is set up. The algorithm operates on the matrices and obtains a low-rank operator that can reconstruct the field values as function of space and time. Dynamic Mode Decomposition obtains an approximate finite dimensional Koopman operator for linear systems. We illustrate the process for simple structures - flat tensile specimen and plate with hole using data obtained from finite element computations and from experiments using Digital Image Correlation. Additionally, we show a thermal system with multiple thermal conductivities using data obtained with an infrared camera. Unsupervised rank truncation is also outlined using the Gavish-Donoho method [2].

In the case of non-linear solids, a special observable function, taken as a neural network here, is learned from the data and an approximate, finite-dimensional Koopman operator is shown to “linearize” the non-linear system of ODEs. The latter allows linear superposition to be used for elastic-plastic solids.

Key contributions in this work are the development of data-driven operators that could serve as reduced-order models for linear and non-linear solids.

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Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING CONTINUUM DAMAGE COUPLED TO PLASTICITY IN PAPER

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ABSTRACT

There is an increasing need, particularly among packaging manufacturers, for simulation tools that can enable efficient structural calculations for paper and cardboard structures. Nevertheless, although the field of application for paper and paperboard is very broad, the modeling of its material behavior – particularly its damage and failure response – has not yet been sufficiently researched [1].

The material behavior of paper is anisotropic and characterized by elasto-plasticity coupled with progressive damage mechanisms, which results in stiffness reduction [2, 3]. The main challenge in describing these phenomena for paper is that model approaches already established for other materials cannot simply be transferred because the underlying physical effects are determined by the intrinsic microstructure of the material. On the microscale, paper is a network consisting of interconnected fibers, which behaves fundamentally differently from the crystal lattice of metals, for example, where dislocations and plastic slip can occur. It is therefore necessary to develop completely new approaches for paper.

In this work, we aim to investigate the damage behavior of paper and develop a numerical modeling strategy that enables an efficient description of the material response, taking into account both anisotropic plasticity and anisotropic damage development. Since large deformations occur during forming processes, the modeling approach should account for large strain kinematics. Further, in order to ensure mesh-independent results, the model is regularized using the enhanced gradient damage approach.

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Imaging-based methods in computational medicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PATIENT-SPECIFIC LONG-TERM SIMULATION OF TRANSCATHETER EDGE-TO-EDGE MITRAL VALVE REPAIR

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ABSTRACT

Mitral regurgitation (MR) is a highly prevalent and deadly cardiac disease affecting over 2% of the global population. Transcatheter edge-to-edge repair (TEER) has emerged as a generally safe and effective treatment option, where the mitral valve (MV) leaflets are clamped together with a clip device. However, long-term outcomes have been suboptimal, largely due to the heterogeneity of the patient population. Moreover, the MV has demonstrated a capacity to remodel in response to sustained changes in homeostasis, and the long-term impact of the permanent TEER device on the mechanics of the MV leaflets has never been studied. In this study, we have developed a patient-specific, predictive simulation of long-term postoperative MV function based primarily on preoperative, standard-of-care clinical imaging data.
We acquired 3D transesophageal echocardiography (TEE) imaging for five patients undergoing TEER, and additional follow-up imaging at 3-months post-repair. Following our previously published methods, we built a full MV apparatus model for each patient, simulated preoperative systolic closure, and predicted the immediate postoperative MV state by implementing 3D models of the TEER device onto the MV leaflets [1]. Next, we used the follow-up imaging data to fit the plasticity rate constant in our MV plasticity model and applied this model to predict the patient's MV leaflet geometry and deformation at 3-months post-repair [2].
In our predictive follow-up simulations, we were able to reproduce key effects of TEER repair at the 3-month time point using our plasticity model when compared to simulations that directly applied the follow-up boundary conditions. We noted substantial changes in MV function over time not only during systolic closure, but also in diastole when referenced to the preoperative diastolic state, indicating strains that are principally induced by permanent distortions in geometry. Specifically, we observed highly compressive circumferential strain on both leaflets in the region of the clip, and slight radial extension in the same region.
Here, we have presented a novel approach for predicting the postoperative state of the MV apparatus at 3 months post-repair using standard-of-care, preoperative clinical imaging alone. Our results, which reveal continued MV plastic deformation in response to TEER, underscore the importance of a long-term view of repair success in the context of MV function and elucidate potential mechanistic drivers of repair failure, which constitute key targets for optimized treatment durability and efficacy.
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Causal discovery and graphical causal models
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GRAPH ATTENTION EMBEDDINGS AS A CAUSAL LENS IN TEMPORAL LINK PREDICTION

Dan Krofcheck[1], Matthew Sweitzer[1], Sarah Simpson[1], Asmeret Naugle[1], Kate Cauthen[1] and Marco Campos[1]*

[1]Sandia National Laboratories

ABSTRACT

Graph representations of complex systems are an incredibly powerful tool for modeling a broad set of domains, with wide adoption seen in application across social networks, behavioral sciences, trade, transportation, logistics, and cyber networks. However, while these state of the art graph representation methods have shown to be performant, they critically lack the ability to contextualize inference in any sort of causal framework, instead relying strictly on correlations to execute tasks such as classification and prediction. Most state of the art solutions leverage algorithms such as graph attention to generate latent representations from both the structural and temporal aspects of change. Those embeddings are then leveraged for downstream tasks, such as classification and prediction. Here, we explore the potential of these latent representations from graph attention based models to serve as a starting point for extracting causal structure from model inference. Specifically, we investigate leveraging the structural and temporal attention coefficients from state of the art models including DySAT and analogous representations in TGN, to propose a mechanism for causal model inclusion in existing link prediction frameworks.

Our initial investigations are focused on the manner in which the embedded relationships change as node or edge attributes are enriched using additional data about the system. For this study, we explore the inclusion of static and temporally evolving exponential random graph model (ERGM) derived node features to structure experiments comparing 1) the predictive potential of the resulting embeddings, and 2) our ability to explain link prediction tasks given the ERGM statistic inclusion in the node representations. Our results here are largely exploratory, with a focus on the conceptual approach and initial demonstration of techniques to extract causal relationships from link prediction tasks in graph attention based embedding models.

Computational methods in environmental fluid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ESTIMATING SURFACE-LEVEL WINDS FOR STORM SURGE SIMULATIONS USING A CYGNSS-INFORMED PARAMETRIC MODELING APPROACH

Aaron Sines[1], Ethan Kubatko[1], Suranjan Nepal[1], Mohammad Al-Khaldi[1] and Younghun Kang[2]*

[1]The Ohio State University
[2]The University of Texas at Austin

ABSTRACT

Many different parametric tropical cyclone (TC) models have been constructed with the intent of providing accurate wind and pressure fields for engineering applications. Regardless of which model is chosen, typical storm characteristics (e.g., intensity and size) are utilized to first generate the so-called gradient winds, i.e., the winds at the gradient height (~300 m above sea level for normal (non-TC) conditions). From there, the constructed gradient winds are adjusted to provide surface-level (=10 m) winds. One simple approach that is often used to make the adjustment from gradient to surface-level winds is the application of a fixed wind reduction factor (WRF); however, such an approach fails to take into account the dependence of the WRF on storm characteristics, as suggested in previous research.

Therefore, in this work, using surface-level wind speed data retrieved from NASA's Cyclone Global Navigation Satellite System (CYGNSS) mission, thirty-six storms, between the years of 2018 and 2022, were analyzed against the gradient winds produced from the classic Holland parametric TC wind model to derive an empirical relationship between the WRF and the storms maximum sustained wind. The derived WRF relationship is implemented into the ADCIRC storm surge model and tested on a number of hurricanes that made landfall on the US East Coast, where the obtained results are compared to the "standard" technique of using a fixed WRF.

Uncertainty quantification and scientific machine learning for predictive modeling of complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CHANCE CONSTRAINED OPTIMAL DESIGN FRAMEWORKS IN THE FACE OF HIGH-DIMENSIONAL UNCERTAINTY

Pratyush Kumar Singh[*1] and Danial Faghihi*[1]

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ABSTRACT

This work introduces computationally efficient frameworks for the optimal design of thermal insulation components of buildings to achieve target insulation performances while retaining sufficient mechanical stability. The thermomechanical behavior of the component is governed by a multi-phase continuum model as partial differential equations (PDE). The model incorporates uncertain parameters related to the elasticity and thermal conductivity of solid and fluid phases, with the spatial distribution of porosity over the insulation components' domain as the design parameter. The design and uncertainty parameters are both space-dependent fields that, after finite element discretization, result in a high-dimensional design problem. To this end, a risk-averse cost functional is employed to achieve both target performances and mitigation of uncertainty during the design process. Additionally, to avoid stress concentration chance constraints are incorporated into the optimization formulation, ensuring that the probability of a certain function exceeding or going below a threshold value. Finally, to promote sparsity in the design solution, a phase-field regularization function is utilized via a continuation numerical scheme. Two efficient and dimension-independent solution algorithms are proposed for the resulting PDE-constrained optimization under uncertainty. The first approach is based on second-order Taylor approximation of the design objective that solves a generalized eigenvalue problem using a randomized algorithm that only requires the action of the Hessian on a small number of random directions. The second approach is based on approximating the PDE solution using a scalable neural operator that reduces the computational cost of the optimization while provides information about the derivative of parameters with respect to the design parameters. The accuracy, efficiency, and scalability of the proposed design under uncertainty frameworks are demonstrated with examples of various building insulation scenarios. The numerical results indicate that using the proposed approximations leads to computational savings up to several orders of magnitude in the optimization solution.

UQ-TTA student paper competition in uncertainty quantification
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CHANCE CONSTRAINED OPTIMAL DESIGN FRAMEWORKS IN THE FACE OF HIGH-DIMENSIONAL UNCERTAINTY

Pratyush Kumar Singh[*1] and Danial Faghihi*[1]

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ABSTRACT

This work introduces computationally efficient frameworks for the optimal design of thermal insulation components of buildings to achieve target insulation performances while retaining sufficient mechanical stability. The thermomechanical behavior of the component is governed by a multi-phase continuum model as partial differential equations (PDE). The model incorporates uncertain parameters related to the elasticity and thermal conductivity of solid and fluid phases, with the spatial distribution of porosity over the insulation components' domain as the design parameter. The design and uncertainty parameters are both space-dependent fields that, after finite element discretization, result in a high-dimensional design problem. To this end, a risk-averse cost functional is employed to achieve both target performances and mitigation of uncertainty during the design process. Additionally, to avoid stress concentration chance constraints are incorporated into the optimization formulation, ensuring that the probability of a certain function exceeding or going below a threshold value. Finally, to promote sparsity in the design solution, a phase-field regularization function is utilized via a continuation numerical scheme. Two efficient and dimension-independent solution algorithms are proposed for the resulting PDE-constrained optimization under uncertainty. The first approach is based on second-order Taylor approximation of the design objective that solves a generalized eigenvalue problem using a randomized algorithm that only requires the action of the Hessian on a small number of random directions. The second approach is based on approximating the PDE solution using a scalable neural operator that reduces the computational cost of the optimization while provides information about the derivative of parameters with respect to the design parameters. The accuracy, efficiency, and scalability of the proposed design under uncertainty frameworks are demonstrated with examples of various building insulation scenarios. The numerical results indicate that using the proposed approximations leads to computational savings up to several orders of magnitude in the optimization solution.

Emerging topology and shape optimization techniques in computational design of materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTIMATERIAL TOPOLOGY OPTIMIZATION WITH PRE-EXISTING INTERFACIAL CRACKS

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ABSTRACT

Topology optimization offers a powerful tool for designing high-performance structures and metamaterials, composed of one or more base materials. However, the distinct elastic and fracture properties of the interfaces can significantly affect the overall behavior of the structure. While traditional SIMP-based topology optimization methods assume perfect interfaces, real-world scenarios often involve pre-existing cracks, which may compromise the fracture resistance of the structure. This work presents a multi-material topology optimization framework that incorporates pre-existing interface cracks into the optimization process. We utilize density smoothing and projection schemes to directly embed information about the location and geometry of cracks, eliminating the need for crack nucleation and growth simulations. The crack length is controlled by the filter parameters. The minimum compliance problem with volume constraint is considered, while an aggregated stress constraint is incorporated to limit the stresses at the crack tip and resist further crack propagation. The gradients of the objective and constraints are computed using the adjoint sensitivity analysis. Results demonstrate the framework's ability to generate optimized structures with significantly improved fracture resistance, in the presence of pre-existing interfacial cracks. This work paves the way for the design of more resilient and damage-tolerant structures in various engineering applications.

New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

OPTIMIZING ROTATING MACHINERIES: A STUDY ON NATURAL FREQUENCY CONSTRAINTS APPLIED IN TOPOLOGY OPTIMIZATION OF FLUID-STRUCTURE INTERACTION PROBLEMS

Lucas Siqueira[*1], Anderson Azevêdo[1], Emílio Silva[1] and Renato Picelli[1]*

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ABSTRACT

In some rotating machinery, the operation assembly presents tight tolerances, leading to wear problems caused by excessive vibrations. In this context, it is crucial to enhance the design of these components to reduce vibration levels and avoid resonant conditions. Based on that, this study focuses on topology optimization for turbulent swirl flow in fluid-structure problems considering natural frequency constraints applied to the 2D axisymmetric solids. The optimization problem proposed is compliance minimization subjected to a volume constraint and a frequency constraint applied to the three lowest natural frequencies. To ensure that the frequencies of interest are properly restricted, the modal assurance criterion-based (MAC-based) mode-tracking method is used to identify mode crossing during the optimization process. The governing equations are solved using separate domains and the k-ω turbulence model with standard wall functions. The optimization method employed is the Topology Optimization of Binary Structures with Geometry Trimming (TOBS-GT), which separates the Finite Element Analysis (FEA) module (COMSOL Multiphysics) from the optimization module (MATLAB), providing more accurate mesh analysis. Compliance sensitivities are computed through automatic differentiation using the adjoint method, while natural frequency sensitivities are derived through automatic differentiation using the forward method. Both sensitivities calculations are provided by a built-in optimization module in COMSOL Multiphysics. Numerical results explore the optimization of 2D axisymmetric solids subjected to a turbulent swirl flow, encompassing the stiffer design of the structure adhering to predefined natural frequency constraints. Three numerical examples are explored to study the design of the rotating wall through topology optimization, considering a Fluid-Structure Interaction (FSI) problem. These examples include the rotating wall, the rotating and stationary wall system, and the stator structure. The results ensure that the method works to increase the natural frequency of structures subjected to a turbulent fluid flow. The optimizer provides stiffer structures ensuring the predefined natural frequency constraint. However, the manufacturing of these structures is complex. Another point is that the wet optimization tends to worsen the fluid flow optimization. Then, a complementary analysis considering the stator as design domain was carried out.

ESTIMATION OF BIOMECHANICAL PARAMETERS IN THE PROSTATE USING PHYSICS INFORMED NEURAL NETWORKS (PINNS)

Arturo Sirvent-Fresneda[*1], Mauricio C. Vanzulli[2], Christian Diaz-Cuadro[2], Enrique Nadal[1], José Manuel Navarro-Jiménez[1], Santiago Gregori[1] and María José Rupérez[1]*

[1]*Universitat Politècnica de València*
[2]*Universidad de la República*

ABSTRACT

In the quest for innovative approaches to tackle soft tissue and organ simulation, Physics Informed Neural Networks (PINNs) emerge as a promising tool. These algorithms provide a novel perspective on solving differential equations by utilizing neural networks to directly approach solutions associated with deformations, as opposed to traditional methods such as the Finite Element Method (FEM). This shift towards artificial intelligence in biomechanical modeling is part of the contemporary evolution in scientific research.

While Finite Element Methods (FEM) have been instrumental in tissue simulation, their applicability may be constrained in demanding scenarios like real time simulations. PINNs, on the other hand, present themselves as an alternative capable of overcoming these limitations by harnessing the neural networks' capacity to learn complex patterns, thus accelerating inference times.

In comparison to conventional data-driven approaches, which often necessitate extensive datasets for model training, we advocate for the utilization of Physics Informed Neural Networks. Our work delves into the potential of PINNs in solving differential equations for soft tissue deformation, with a particular focus on organs like the prostate. It examines how these neural networks can guide resolution based on underlying physical laws for both the direct and inverse problems, enabling faster and more efficient estimation of biomechanical parameters, turning them into trainable parameters of the network.

This research aims to advance the understanding and modeling of biomechanical phenomena, emphasizing its real-world application for tissue, and promoting the application of PINNs as an effective tool in this context, for future real-time and geometry-free soft tissue simulations in a clinical work environment.

Recent advances in numerical methods for mixed-dimensional PDEs
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INTRINSIC MULTI-DIMENSIONAL ELASTIC COUPLING VIA ENRICHED CONTINUA

Adam Sky[1], Jack S. Hale[1], Andreas Zilian[1], Stephane Bordas[1] and Patrizio Neff[2]*

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[2]*University of Duisburg-Essen*

ABSTRACT

The problem of coupling multi-dimensional continua in a single computational model is commonplace in structural analysis, where one-dimensional models such as Timoshenko-Ehrenfest beams, two-dimensional models such as Reissner-Mindlin plates [1], and the full Cauchy-continuum are coupled to represent one structural design. Although solutions do exist, for example via intermediate finite elements, or more recently with mortar approaches [2], these require either a sophisticated adjustment of the computational domain or modifications of the original problem, e.g., via Lagrange multipliers. In this work we present an alternative approach by employing a mathematically enriched continuum model [3]. The kinematical reduction of the model to lower dimensional domains leaves its fundamental degrees of freedom intact. Consequently, the degrees of freedom intrinsically agree even at the interface with a domain of a different dimensionality. We introduce the derivations of all models of various dimensions, present applications with numerical examples, and conclude the talk with an outlook on possible future developments.

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Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPING A FRACTURE PROBABILITY CURVE BASED ON OBSERVABLE MICROSTRUCTURE IN ADDITIVELY MANUFACTURED CERAMICS

Elizabeth Smith[*1]*

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ABSTRACT

Accurately predicting fracture of additively manufactured ceramics is an essential step to their adoption in industrial and other high precision environments. As a relatively young innovation, there is high variability in manufacturing techniques, potential base materials, and subsequent mechanical properties of additively manufactured ceramics. However, additive manufacturing can create high precision geometries impossible with conventional methods that have potential applications in fields such as aerospace and biomedical engineering. In addition to the variability between components, additive manufacturing can introduce anisotropy as a consequence of layer deposition methods. We developed a method to use statistics based on observable microstructural properties, including pore and grain size distributions, to estimate a fracture probability distribution under a prescribed loading in an anisotropic material. The entire process from model creation to microstructural analysis to development of the fracture distribution curve will be demonstrated.

Microstructure data is taken from SEM images of relevant samples. Image processing techniques and EBSD are then used to generate profiles for grain and pore geometry distributions. This data is then used to inform strength variations for an anisotropic material based on methods presented by Takeo et al (2019) and Gavazzi and Lagoudas (1990). Using FEA, a stress field is obtained and compared to the strength distribution to generate a failure of probability under a given loading. This method can be applied to any geometry and loading. This workflow enables relatively rapid and efficient prediction of fracture using observable properties of an individual sample.

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UNCERTAINTY ANALYSIS IN THE PRESENCE OF MODEL-FORM ERRORS

Ralph Smith[*1]*

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ABSTRACT

Model discrepancies, or model-form errors, can dominate parameter and observation error uncertainties for many models. These errors are generally epistemic, rather than aleatoric, and can significantly diminish the sole reliance on statistical analysis when calibrating models for subsequent predictions. Moreover, unaccommodated model discrepancy can significantly diminish the accuracy of prediction intervals for model responses and limit the degree to which they can be employed for model validation. Whereas solely data-driven techniques can be effective for certain interpolatory predictions, they generally fail when extrapolating outside the data, which is the case when predicting future behavior using time-dependent models. In this presentation, we will detail some of these issues and discuss techniques to quantify model discrepancy to improve the accuracy of extrapolatory predictions and uncertainty analysis. This generally relies on identifying and improving the accuracy of model components determined to be producing epistemic errors. We illustrate these techniques using a variety of models having highly nonlinear parameter dependencies.

AN APPROACHABLE PROBLEM FOR THE BAYESIAN ANALYSIS OF A VARIETY OF UNCERTAINTIES IN HIERARCHICAL PHYSICAL MODELS

Sean Smith[*1], Giridhar Gopalan[1] and Devin Francom[1]*

[1]*Los Alamos National Laboratory*

ABSTRACT

This presentation will introduce a simplified model of an industrial fixed-bed ethylene-oxide reactor with coupled sub-models for: particle-film mass transfer, pore diffusion, turbulence & reaction kinetics. The analysis will also account for experimental data corresponding to a subset of the sub-models as well as pilot-scale data for the coupled system. We will discuss the interaction of various sources of uncertainty, such as: parameter uncertainty, model-form uncertainty, surrogate-model/emulator uncertainty, experimental uncertainty, instrument-model uncertainty and prediction-scenario uncertainty. The meaning of the words aleatory & epistemic within a Bayesian context will be briefly addressed. Various techniques from the Bayesian UQ literature for handling the complicating sources of error will be presented in the context of this model, such as: emulation, dimension reduction, parameterizing a model's output errors into its inputs, identification & propagation of discrepancy (model-form error) for the sub-models, and feedback cutting.

Multiscale computational and data-driven approach of advanced materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFICIENT COMPUTATIONAL MULTISCALE ANALYSIS FOR THE HOMOGENIZATION OF NONLINEAR SOLIDS USING SAMPLING STRATEGIES OF MICROSCOPIC MODELS

Yujin So[*1], Suhan Kim[2], Hyunseong Shin[2] and Jaehun Lee[1]*

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ABSTRACT

In this study, we introduced the model order reduction method at the microscale level to improve the computational efficiency of the multiscale finite element analysis. Recently, various industrial applications have been using multi-scale analysis that reflects the characteristics of microstructures to predict the behavior of structures made of composite materials. Among the several multiscale analyses, the multiscale finite element analysis is one that analyzes the macroscale equivalent structure through the microscale analysis, which solves the two-scale boundary value problem. This method performs repetitive computations of the microscopic self-equilibrium equation at every integration point in the macroscale structure. Therefore, we require high computational costs. A significant amount of computational resources is especially required for the multiscale analysis, considering the nonlinearities in both macro and microscopic domains. Thus, in this study, we applied the reduced-order model technique to reduce the computation time of multiscale finite element analysis considering the nonlinearities.
We propose introducing reduced-order modeling of the representative volume element model in microscale using nonlinear reduced-order modeling to improve the efficiency of multiscale finite element analysis. We obtain the computational efficiency in the online stage. Since the unit cell deforms according to the macroscale strain, we derive a reduced-order model corresponding to the macroscale strain. Significantly, the size of the reduced-order model used to simulate a wide range of deformation can be large, which affects computational efficiency, so we conducted research to reduce its size. In the offline stage, we construct the reduced-order model of representative volume element through full-order representative volume element model analysis. Then, we perform the multiscale finite element analysis in the online stage using the reduced-order model of representative volume element. We verify the proposed method comparing accuracy and efficiency with those of full multiscale finite element analysis investigating microscopic and associated macroscopic models.

Advanced discretization schemes and solution strategies for computational structural dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN ENHANCED FULLY-ADAPTIVE EXPLICIT-IMPLICIT TIME-MARCHING FORMULATION FOR ELASTODYNAMICS

Delfim Soares[1], Lucas Pinto[2], Isabelle Sales[2] and Webe Mansur[2]*

[1]*Federal University of Juiz de Fora*
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ABSTRACT

In this work, an explicit-implicit time-marching formulation, which adapts to the model's properties, its adopted spatial and temporal discretizations, and its computed responses, is studied for elastodynamic analyses. Explicit-implicit approaches have become referred to as effective time-domain solution methodologies since they allow combining the advantageous features of both explicit and implicit formulations, such as reduced solver efforts and guaranteed stability, providing very attractive techniques. The here discussed time-domain hybrid solution procedure is based on three simple single-step recurrence relationships, which are formulated considering three locally-defined time-integration parameters, namely α_0^e, α_1^e and α_2^e, and each one of these time-integration parameters is adaptively determined for each element “e” of the adopted spatial discretization. In this context, the α_0^e parameter distinguishes explicit ($\alpha_0^e=0$) and implicit ($\alpha_0^e\neq0$) elements, while α_1^e and α_2^e delineate non-dissipative ($\alpha_1^e=\alpha_2^e=0$) and dissipative ($\alpha_1^e\neq0$ and $\alpha_2^e\neq0$) elements. The adopted non-null expression for α_0^e ensures that, in the absence of numerical dissipation, the critical sampling frequency of the method aligns with the maximum sampling frequency of the element, allowing the element to operate as if provided with its critical time-step value. This configuration not only ensures stability, but also better counterbalances the errors of the considered temporal and spatial discretization procedures, enhancing the overall accuracy of the computed discrete solution. On the other hand, the non-null expressions that are defined for α_1^e and α_2^e are designed to set the bifurcation sampling frequency of the method equal to the maximum sampling frequency of the element and its bifurcation spectral radius to zero. This configuration maximizes numerical dissipation for the element's maximum sampling frequency, effectively dissipating spatially unresolved high-frequency modes while accurately evaluating important low-frequency modes, since the developed adaptive formulation ensures that dissipative elements are activated only when and where it is necessary in the analysis. In addition, an optimal time-step value for maximal computational efficiency is also evaluated in the proposed solution methodology, based on the “particle swarm optimization” algorithm, which minimizes the expected total number of operations in the hybrid solution process. In this case, the optimal time-step value is determined so that the most efficient distribution of explicit and implicit elements is considered in the analysis, providing a highly effective, fully-adaptive and entirely automated, time-domain solution procedure. At the end of this work, numerical results are presented and compared to those of standard time-marching procedures, demonstrating the excellent performance of the reported adaptive hybrid approach.

New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION FOR FLUIDIC DIODE DESIGN WITH DISSIPATION AND VORTICITY FUNCTIONS VIA SEQUENTIAL APPROXIMATE INTEGER PROGRAMMING

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ABSTRACT

Recent advancements in computational tools and additive manufacturing have expanded design possibilities on fluid devices to industrial applications. In this context, gas fluidic diodes emerge as a potential sealing mechanism to guarantee rotating machinery performance and reduce environmental pollution. In this study, novel trends in topology optimization applied to fluidic diode design are explored. We propose cutting-edge strategies to address challenges observed in traditional fluid flow optimization procedures. The main challenges for labyrinth seal designs are: i) physical modeling for moderate and high fluid flow speed, ii) bad local minimum of fluid inlet/outlet closure, iii) absence of interlocked labyrinth-like solid regions, and iv) capture the main dissipative effects produced by flow recirculation and throttling along the two-dimensional axisymmetric geometry in a suitable objective function. We demonstrate the TOBS (Topology Optimization of Binary Structures) method potential to provide innovative designs and solve each of the discussed issues. One of the advantages of this discrete approach is the explicitly defined domains during the entire optimization due to the absence of intermediate density values (e.g., gray-scale region), consequently easing the prototypes manufacturing and allowing surface tracking (useful to apply design-dependent boundary conditions). In order to provide a comprehensive guideline for the labyrinth seal geometry dissipative effects for low to high flow regime: energy dissipation, vorticity, and flow velocity components are investigated as single and multi-objective expressions. The sensitivity field of objective functions is computed via automatic differentiation. Fluid flow volume or the minimum gap between the stationary and rotatory solid phases is chosen as the constraint function according to the example. In our approach, the fluid flow governing equations are solved using the Finite Element Method and the optimization problem via Integer Linear Programming. The problem discretization is performed using regular mesh on jagged patterns assuming a laminar regime and adaptive smoothed boundary fitting mesh assuming turbulence wall models.

Advances in discretization techniques, element technology, mesh adaptivity, and solution strategies for inelasticity, localization, and failure
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN AUTOMATED COMPUTATIONAL FRAMEWORK RELYING ON A NON-ITERATIVE MESHING ALGORITHM FOR MODELING MATERIALS WITH COMPLEX MICROSTRUCTURES

Soheil Soghrati[1], Salil Pai[1], Pengfei Zhang[1], Balavignesh Vemparala[1] and Kartik Kashyap[1]*

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ABSTRACT

An integrated computational framework relying on virtual microstructure reconstruction and parallel mesh generation algorithms will be presented to simulate the multiscale failure response of composite materials. A virtual reconstruction algorithm is developed to synthesize various material microstructures, particulate, fiber-reinforced, and woven textile composites. This approach first employs a virtual packing algorithm to build an initial microstructural model with arbitrary-shaped embedded fibers/particles, followed by a reduced-order finite element (FE) compaction simulation to synthesize microstructures with densely packed inclusions. A genetic algorithm (GA) based optimization phase is then utilized to replicate target statistical microstructural descriptors such as the volume fraction, spatial arrangement, and orientations of embedded inclusions. Unlike most reconstruction algorithms, the output of this algorithm is presented in the form of NURBS patches or STL files to represent material interfaces for the subsequent mesh generation explicitly.

Conforming FE meshes for the resulting complex material microstructures are generated using a non-iterative, parallel meshing algorithm, coined Conforming to Interface Structured Adaptive Mesh Refinement (CISAMR). The CISAMR algorithm automatically transforms a structured background grid into a high-quality tetrahedral conforming mesh using customized h-adaptivity, r-adaptivity, element-deletion, and sub-tetrahedralization algorithms. We present several new algorithmic features of the CISAMR, including a Kirigami-inspired algorithm for efficient sub-tetrahedralization of background elements, handing material interfaces with sharp edges/corners, and modifications to automatically handle resin interstices and yarn interpenetrations (an artifact of the compaction phase of the microstructure reconstruction process) in woven textile composites. In addition to the application for meshing composite material microstructures, we discuss expanding the CISAMR algorithm for modeling polycrystalline microstructures and crack growth problems. Various example problems are provided to demonstrate the application of this reconstruction-meshing framework for modeling real-world materials systems.

Advanced model order reduction techniques for computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

META-MODELS PREDICTING GAS DYNAMIC PERFORMANCE OF A HYDROGEN RE-CIRCULATION EJECTOR IN A FUEL CELL SYSTEM

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ABSTRACT

As a climate crisis is recognized as one of the most important issues on global economy, eco-friendly vehicle systems have become a new trend among global vehicle manufacturing companies. Instead of a high-performance and low-emission internal combustion engine, full electric vehicles powered by lithium-ion batteries have been considered to be the next automobile system in the near future. This can be proved by the fact that the number of customers seeking electric vehicles has increased. Hydrogen fuel-cell vehicles are also electric-powered vehicle system, however, there is a significant difference in electricity generation between lithium-ion batteries and fuel-cells. Since fuel-cells consume hydrogen and oxygen to generate electricity, and the hydrogen gas has low density compared to the oxygen or other gases, it must be treated very carefully. In other words, a hydrogen gas ejector supplying the hydrogen gas into the fuel-cell system needs to be precisely designed.

This work discusses a meta-modelling and optimization process with respect to the design parameters of the hydrogen re-circulation ejector to predict the gas dynamic phenomena inside the ejector. The hydrogen re-circulation system means that the hydrogen gas which remains after being consumed in the fuel-cell module is returned to the ejector. Re-circulation ejector enables the hydrogen gas to be efficiently worked for the generation of electricity in the fuel-cell. Computational fluid dynamic (CFD) analysis based on finite volume discretization is adopted to simulate the hydrogen gas flow inside the ejector. Some of design parameters which significantly influence the re-circulation rate, a key performance of the hydrogen ejector, are selected. Combinations of design variables are finally sampled using a design of experiments (DoE) and gas flow simulations are made for each set of design variables.

Mathematical formulations in terms of design variables for predicting the performance of the hydrogen re-circulation ejector are derived by meta-modeling techniques. The coefficients of prognosis (CoP) from the derived meta-models and the sensitivity of design variables are examined. The meta-model with the best accuracy is used to determine the final design variables that allow the best performance of the ejector. Through these meta-models and optimization processes, the initial design of the hydrogen gas ejector, which supplies the hydrogen gas into the fuel-cell system, would be noticeably improved.

Multiscale topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MICRO AND MACRO SCALE TOPOLOGY OPTIMIZATION OF MULTI-MATERIAL FUNCTIONALLY GRADED LATTICE STRUCTURES

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ABSTRACT

Lattice structures are gaining popularity as a favored design approach across various engineering applications. The growing appeal is primarily attributed to their high specific strength and stiffness, effective heat dissipation, and relatively lightweight nature, among other advantages. The use of additive manufacturing techniques has allowed for increased flexibility and resolution, leading to the development of more detailed and better-performing lattice structures. Material unit cell designs without restrictions are frequently linked to challenges such as high computational demands and connectivity issues. On the other hand, highly constrained lattice unit cell designs, despite their lower computational cost, may not attain the optimal desired properties.

This study aims to enhance the flexibility of a restricted unit cell design while maintaining a lower computational cost. The approach involves a two-scale concurrent optimization of the lattice structure, simultaneously optimizing the topology at both macro and micro scales to attain an optimal configuration. To ensure a continuous optimization process, surrogate models are employed to define material and geometrical properties. The elasticity tensors for a lattice unit cell are derived using an energy-based homogenization method combined with voxelization. A multi-variable parameterization of the material unit cell is established to enable the synthesis of functionally graded lattice structures. Therefore, the compliance is considered as the objective function, while relative density and aspect ratio are two key design variables. The proposed topology optimization framework is employed for different case studies.

Multi-physics and multi-scale simulations with the coupling library preCICE
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

OVERVIEW OF MULTIPHYSICS COUPLING EFFORTS AT LLNL FOR ADVANCED ENERGY APPLICATIONS

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ABSTRACT

Various multiphysics coupling efforts exist at LLNL aimed at advanced energy applications. An ongoing effort has coupled the LLNL multiphysics code Diablo to Nek5000 focused on various fluid-structure interaction applications emanating from such applications. This effort has largely used bespoke coupling algorithms within Diablo and Nek5000. A more recent set of work has coupled OpenFOAM and Diablo in the context of coupled thermofluid/structural calculations, with a more nascent effort to also include electromagnetic effects. We discuss the relative merits of different approaches along with the ongoing challenges and future work.

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Complex fluid flows in engineering: Modeling, simulation, and optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING A PULSATILE SHEAR-THINNING 2D CHANNEL FLOW WITH PHYSICS-INFORMED NEURAL NETWORKS.

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ABSTRACT

Our study delves into the investigation of shear-thinning fluid flow, which is common in various industrial applications such as transport of battery slurries or usage of polyacrylamide solutions in heavy oil recovery. Specifically, the focus is on pulsatile shear-thinning flows through a straight channel. While previous studies have relied on traditional methods such as the finite element method to study the topic [1], this study introduces the use of physics-informed neural networks (PINNs) as a novel approach to solve the complex fluid flow. Since its inception, PINNs have been successfully employed to model a diverse range of fluid flow problems, including modeling a time-dependent flow around a cylinder [2], or simulation of steady-state flows in channels of varying width [3].

To ensure an accurate simulation of the time-dependent shear-thinning flow, we optimized the hyperparameters of the PINN model such as implementation of the boundary conditions, neural network structure, number of training points, and loss weights in the loss function. This optimization process was carried out through a series of case studies, each supplemented with Gaussian processes-based Bayesian optimization. The findings suggest that augmenting the number of training points is more beneficial than using large networks for the problem at hand. Additionally, the use of swish activation, hard-REQ constraints for boundary condition enforcement, and assigning large loss weights for the continuity loss term significantly improves the model's performance. A good agreement is achieved between the reference solution and the finalized PINN model, indicating that properly trained PINNs can be used as effective surrogates for simulating pulsatile shear-thinning flows.

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Advances and applications of polytopal methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A SCALED BOUNDARY FINITE ELEMENT FRAMEWORK TOWARDS FULLY AUTOMATED ENGINEERING ANALYSIS

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ABSTRACT

A scaled boundary finite element framework towards fully automated engineering analysis

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The process of computational engineering analysis includes the discretization of geometric models and the solution of partial differential equations using numerical methods. In the popular finite element method, a geometric model is discretized into a mesh of elements of simple geometries (triangles and quadrilaterals in 2D, and tetrahedrons and hexahedrons in 3D). With increasingly affordable computer power, the human effort required in mesh generation becomes increasingly critical in terms of both cost and time. Furthermore, geometric models in digital image, STL format and point clouds are becoming more and more popular in engineering applications and present challenges to well-established numerical methods.

This presentation covers the development of the scaled boundary finite element method [1], aiming to fully automate the process of engineering analysis directly from common formats of geometric models. The scaled boundary finite elements require the discretization of boundary only and can have any number of faces, edges and vortices, leading to a much higher degree of flexibility in mesh generation than standard finite elements. This allows the use of simple and efficient quatree/octree algorithm for fully automatic mesh generation of digital images, STL models, point clouds and traditional CAD models in a unified approach. Moreover, the algorithm is suitable to high-performance computing (HPC) [2]. Some salient features and HPC performance of the proposed technique will be demonstrated by numerical examples.

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Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT OF A CELL-BASED MATERIAL POINT METHOD AND CONTACT TECHNIQUE

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ABSTRACT

Recently, particle-based methods have been developed to overcome the limitations of the FEM. Among these particle-based methods, the material point method (MPM) has been proposed to efficiently solve large deformation problems by combining the advantages of Lagrangian and Eulerian descriptions of motion. In the MPM, the continuum is discretized into material particles carrying all state variables, and the weak form of the governing equations is solved on a background grid. Since the deformation field of the MPM is computed on a background grid, element distortion and mesh entanglement in the FEM do not occur in the MPM simulation of large deformation problems. Using the advantages of the MPM, it has been applied to solve problems with complicated deformations, crack propagation, contact and fluid-solid interactions.

Although the MPM has an ability to solve large deformation problems, the error caused by cell crossing of material particles and the error in numerical integration of the weak form lead to the degradation in the performance of the MPM. The cell-crossing error occurs when material particles cross the grid cell boundaries due to the lack of smoothness of the piecewise linear shape functions defined on a background grid. Several studies have been carried out to reduce the cell-crossing error by replacing the piecewise linear shape functions with other smooth functions. Another important issue in the MPM is that the accuracy of numerical integration of the weak form can be poor and fluctuating in the spatial domain when material particles are unequally placed over a background grid.

In this study, a new cell-based integration scheme is developed to improve the convergence of implicit MPM computations for large deformation static problems and eliminate cell-crossing errors. The increment weak form based on the updated Lagrangian approach is formulated for the implicit MPM. In order to eliminate the cell-crossing error and to reduce the integration error, numerical integration of the incremental weak form is performed on grid cells. Additionally, a nodal volume-based boundary definition method is developed to apply contact boundary conditions to cell-based MPM. A contact analysis technique using the penalty method is developed using boundaries defined in the background grid.

Microstructures of chemically complex materials and their impacts on material properties from multiscale simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INTRINSIC DEFORMATION ASYMMETRY FROM SYMMETRY BREAKING IN ORDERED INTERMETALLIC ALLOYS: ATOMISTIC ORIGINS AND CONTINUUM MODELING

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ABSTRACT

We have performed a comprehensive investigation of symmetry breaking in the interactions between dislocation and various superlattice planar faults in intermetallic alloys, to reveal the underlying dislocation mechanisms that govern intrinsic plastic deformation asymmetry, employing both large-scale atomistic simulations and continuum dislocation theory. Ni-based and Ti-based alloys, of different crystal structures, were examined, with two primary symmetry breaking effects, i.e., translational and three-fold rotational symmetry breaking considered. Detailed asymmetrical dislocation reactions and the corresponding dislocation bypassing mechanisms have been elucidated, shown to be highly dependent on the geometrical configuration of the precipitate and the relative magnitudes of fault energies. A continuum model framework was then developed, which, for the first time, provides accurate and quantitative predictions of the threshold conditions triggering critical asymmetrical dislocation slips, verified to be in good agreement with the simulation results. The findings provide critical new understanding of deformation asymmetry in intermetallic alloys.

Uncertainty quantification and reliability analysis in engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATION OF WORST-CASE LOAD UNCERTAINTY IN INDUSTRIAL ROBOTS DESIGN OPTIMIZATION

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ABSTRACT

Facing various application scenarios, industrial robots need to perform multiple different trajectories, or cycles. At the same time, in order to improve the payload-to-weight ratio and reduce energy consumption, it is necessary to lightweight the robot as much as possible while fulfilling the requirements of multiple cycles. Hence, the optimal design of the industrial robot structure still faces many challenges, such as the high computational cost required for analyzing and optimizing the different robot configurations corresponding to different cycles. In this paper, the nominal value and variation of loads (including forces and moments) are defined to represent the deterministic part and uncertain part of the loads respectively, serving as a method to describe the uncertainty of the robot loads. On the other hand, during implementation of cycles by industrial robots, the loads on each link change over time continuously. By employing inverse dynamics, loads that vary with time can be calculated on all joints and joints. These time-varying loads are converted into a nominal value and a variation via time-domain calculations, thus converting the time-varying loads under different robot cycles into an uncertainty. Subsequently, by computing the worst-case loads scenario on robot links, the magnitudes and directions of the worst-case loads under the current structural design and load uncertainty can be determined, along with the calculation of their sensitivities. Furthermore, a comparison is completed between the unidirectional maximal load method and the proposed method for calculating the worst-case loads, and then it is followed by stress analysis using the respective loads and to demonstrate the effectiveness of this new method. Finally, the new method is applied to a typical robot link topology optimization as an example, and the results are compared with the counterpart exploiting the unidirectional maximal load method.

Machine learning algorithms for accelerating material characterization, discovery, design, and manufacturing processes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

REVEALING MICROSCOPIC DYNAMICS: IN-SITU LIQUID-PHASE TEM FOR LIVE OBSERVATIONS OF SOFT MATERIALS AND QUANTITATIVE ANALYSIS VIA DEEP LEARNING

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ABSTRACT

In various domains spanning materials synthesis, chemical catalysis, life sciences, and energy materials, in-situ transmission electron microscopy (TEM) methods exert a profound influence. These methodologies enable the real-time observation and manipulation of gas-phase and liquid-phase reactions at the nanoscale, facilitating the exploration of pivotal reaction mechanisms. Fundamental research areas like crystal nucleation, growth, etching, and self-assembly have greatly benefited from these techniques. Additionally, their applications extend across diverse fields such as catalysis, batteries, bioimaging, and drug delivery kinetics.

However, the intricate nature of 'soft matter' presents a challenge due to the unique molecular properties and dynamic behavior of these substances that remain insufficiently understood. Investigating soft matter within in-situ liquid-phase TEM settings demand further exploration and advancement compared to other research domains. This research harnesses the potential of in-situ liquid-phase TEM technology while integrating deep learning methodologies to comprehensively analyze the quantitative aspects of soft matter dynamics.

This study centers on diverse phenomena, encompassing surfactant molecule nucleation, block copolymer behavior, confinement-driven self-assembly, and drying processes. Furthermore, deep learning techniques are employed to precisely analyze Ostwald ripening and digestive ripening dynamics. The outcomes of this study not only deepen the understanding of soft matter at its fundamental level but also serve as a pivotal foundation for developing innovative functional materials and cutting-edge devices.

Keywords: liquid phase TEM, big data, block copolymer, self-assembly, deep learning,

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Numerical methods, mathematical modeling and analysis in material science
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

REDUCED ORDER MODELING OF A FRICTION STIR WELDING PROBLEM

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ABSTRACT

The friction stir welding process can be modelled using a system of heat transfer and Navier-Stokes equations with a shear-dependent viscosity. Finding numerical solutions of this system of nonlinear partial differential equations over a set of parameter space, however, is extremely time-consuming. Therefore, it is desirable to find a computationally efficient method that can be used to obtain an approximation of the solution with acceptable accuracy. In this talk, we present a reduced basis method for solving the parametrized coupled system of heat and Navier-Stokes equations using a proper orthogonal decomposition (POD). In addition, we apply a machine learning algorithm based on an artificial neural network (ANN) to learn (approximately) the relationship between relevant parameters and the POD coefficients. Our computational experiments demonstrate that substantial speed-up can be achieved while maintaining reasonable accuracy.

Computational methods in environmental fluid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL SIMULATION OF MULTIPHASE FLOW IN POROUS MEDIA

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ABSTRACT

Modeling the flow of liquid, aqueous, and vapor phases through porous media is a complex and challenging task that requires solving nonlinear coupled partial differential equations. In this talk, we propose a second-order accurate and energy-stable time discretization method for the three-phase flow problem in porous media. We prove the convergence of the subiterations to resolve the nonlinearity, and show that the time-stepping method mimics the energy balance relation that the continuous problem satisfies. Our spatial discretization uses an interior penalty discontinuous Galerkin method, for which we establish the well-posedness of the discrete problem and provide error estimates under certain conditions on the data. We validate our method through numerical simulations, which show that our approach achieves the expected theoretical convergence rates. Furthermore, the numerical examples highlight the advantages of our time discretization over other time discretizations.

Fluid-structure interaction: Methods and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL MODELLING OF FRAGMENT AND BLAST LOADED CONCRETE STRUCTURES USING MASSIVELY-PARALLEL COUPLED CFD-CSD TECHNIQUES

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ABSTRACT

This paper describes the numerical formulation of a state-of-the-art coupled computational fluid dynamics (CFD) and computational structural dynamics (CSD) methodology, to the simulation of steel case fragmentation and explosively loaded reinforced concrete structures.

ASI (Applied Simulations Inc.) have developed a numerical methodology that couples state-of-the-art CFD and CSD methodologies [1]. The flow (CFD) code solves the time-dependent, compressible Euler and Reynolds-Averaged Navier-Stokes equations. The CSD code solves the large deformation, large strain, solid dynamic equations on an unstructured grid composed of bricks and tetrahedral elements. VMS (variational multi-scale) stabilization is utilized to improve the robustness and stability of the numerical CSD solution. The codes are coupled via a ‘loose coupling’ approach which decouples the CFD and CSD sets of equations and uses projection methods to transfer interface information between the CFD and CSD domains. Both codes are parallelized using a hybrid MPI/OpenMP methodology. The final presentation will describe in detail the implementation of the concrete fracture, weapon fragmentation and contact algorithm on the mentioned MPI/OpenMP parallelization frame, which allows spectacular simulation speed-up for real life applications. An improved first principles fragmentation scheme, which enforces mass conservation and compare very well qualitatively and quantitatively with experimental results (fragments size distribution), will be shown too.

Finally, a steel case weapon simulation inside a reinforced concrete structure is shown to demonstrate the overall scheme. The simulation addresses the steel case fragmentation, air blast and fragments impact on the concrete structure, structural response, structural failure, debris launch, and propagation of air blast to the far field. The predicted structural disassembly agrees well with the high-speed photography. The predictions exhibit similar failure mechanisms, failure locations and times of failure. The initial structural debris, the weapon fragmentation size distribution, and the weapon fragment velocities follow the experimental ones too. The far field pressures exhibit similar decay with range as the experimental data.

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DEEP CONVOLUTIONAL ARCHITECTURES FOR UNCERTAINTY QUANTIFICATION AND FORECAST IN INUNDATION PROBLEMS

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ABSTRACT

Most science and engineering problems are modeled by time-dependent and parametrized nonlinear partial differential equations. Their resolution with traditional computational methods may be too expensive, especially in the context of predictions with uncertainty quantification or optimization, to allow for rapid predictions. In this talk, we will overview data-driven methods aimed at representing high-fidelity computational models by means of reduced-dimension surrogate ones. Different approaches will be presented for the uncertainty quantification for reliable predictions and forecasts in inundation problems.

Particularly, a non-intrusive reduced-order model based on convolutional autoencoders is proposed as a data-driven tool to build an efficient nonlinear reduced-order model for stochastic spatiotemporal large-scale physical problems. The method uses two-level autoencoders to reduce the spatial and temporal dimensions from a set of high-fidelity snapshots collected from an in-house high-fidelity numerical solver of the shallow-water equations. The encoded latent vectors, generated from two compression levels, are then mapped to the input parameters using a regression-based multilayer perceptron. The accuracy of the proposed approach is compared to the linear reduced-order technique-based artificial neural network (POD-ANN) on benchmark tests (the Burgers and Stoker's solutions) and a hypothetical dam-break flow problem over a complex bathymetry river. The numerical results show that the proposed nonlinear framework presents strong predictive abilities to accurately approximate the statistical moments of the outputs for complex stochastic large-scale and time-dependent problems, with low computational cost during the predictive online stage.
The challenge that remains is the long-term temporal extrapolation for problems marked by sharp gradients and discontinuities. Our recent studies explore forecasting convolutional architectures in space and time (LSTM, TCN, CNN, Self-Attention, and Transformers) to obtain accurate solutions for time-steps distant from the training domain, on advection-dominated test cases. To evaluate the epistemic uncertainties in the predicted solutions, the methodology of deep ensembles is adopted.

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COMPARISON OF REISSNER-MINDLIN AND KIRCHHOFF-LOVE THEORIES BY A SIMPLE NONLINEAR SHELL TRIANGULAR ELEMENT

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ABSTRACT

In solid mechanics, shells are a particularly important model because many structures in engineering can be associated with them: sheet metal products, slabs, thin-walled pressure vessels and other objects with one of their dimensions significantly smaller than others. The Shell models can be adapted for finite element use, but it is important to consider peculiarities such as locking behaviour.
The objective of this work is to examine the behaviour of a nonlinear formulation for shell models using a new displacement-based triangular shell element with 6 nodes. The formulation of the element is implemented in both Reissner-Mindlin and Kirchhoff-Love kinematic assumptions and an initial plane reference configuration for the shells.
The proposed formulation also accounts for finite strains, large displacements, and rotations. The rotation field has been re-parameterised using the Rodrigues rotation vector, resulting in a simpler update of rotational variables.
The computational implementation of the new elements is achieved through automated finite element methods, with some numerical examples. Furthermore, a comparison between these numerical examples and both theories is performed.

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Advanced numerical techniques for fluid flow in porous media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PRECONDITIONERS BASED ON MULTISCALE DOMAIN DECOMPOSITION METHODS FOR POROUS MEDIA FLOWS

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ABSTRACT

Multiscale domain decomposition methods have already shown great scalability in parallel high-performance simulations of heterogeneous subsurface flows [1] at the cost of accuracy compared to the solution of the undecomposed discretizations. In order to take advantage of the excellent scalability properties of multiscale methods without the loss of accuracy, we introduce a family of preconditioners based on multiscale domain decomposition methods for solving heterogeneous single-phase subsurface flows. We build the preconditioners using the Multiscale Robin Coupled Method - MRCM [2], a domain-decomposition method based on the imposition of Robin-type boundary conditions on each subdomain. Depending on the choice of the Robin parameter, the MRCM can reproduce the results of other well-known multiscale methods within the same framework, directly affecting the performance of the resulting preconditioner. This method is combined with iterative linear solvers, such as the Preconditioned Conjugate Gradient method, to solve the linear systems arising from the (undecomposed) Finite Volume discretization of heterogeneous porous media flows. The results show that multiscale methods can be successfully used as preconditioners to improve efficiency when combined with different smoother methods, reducing the number of iterations. Results also demonstrate the flexibility of the MRCM preconditioners as a viable alternative compared to other existing techniques.

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Advanced analysis of steel and steel-concrete composite structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DYNAMICS OF PRESTRESSED STEEL-CONCRETE COMPOSITE MEMBERS

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ABSTRACT

Composite steel-concrete beams may improve their mechanical behavior through application of post-tensioning, allowing longer spans, a larger elastic range and better fatigue behavior, either as building elements or after strengthening/repair. A particular characteristic of composite beams is the possibility of slip or partial interaction between the components as a result of the flexible connection between steel and concrete. Several studies have dealt with these elements recently, but very few addressed the dynamic analysis of such members.
The purpose of this work is to present a numerical scheme for the dynamic analysis (modal analysis, free and forced vibration) of posttensioned steel-concrete composite beams under nonlinear material and geometrical assumptions, considering also partial interaction. The numerical model employs beam-column elements for the steel and concrete sections and a tendon element for the prestressing, taking into account the variation of the tendon stiffness in a consistent fashion. The robustness of the numerical procedure is assessed by means of some examples and parametric studies.

Modeling and simulation of dynamics, stability and control of aerospace structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INVESTIGATING THE DOMAIN OF ATTRACTION OF SDRE APPLIED TO A CUBESAT ATTITUDE CONTROL SYSTEM DURING LAUNCH ORBIT PHASE BASED ON COLD GAS THRUSTERS

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ABSTRACT

The precision of controlling the attitude of a CubeSat during the injection phase in orbit is of fundamental importance for the success of the mission. In general, the CubeSat starts this phase with high angular velocity, and then the controller needs to maneuver the CubeSat to its nominal mode of operation, which is characterized by an attitude of small angles. One way to achieve such a transition between these two modes is by using cold gas thrusters. In this paper, we investigate the Domain of Attraction of State-Dependent Riccati Equation (SDRE) applied to the Attitude Control System (ACS) algorithm during Launch and Early Orbit Phase which has nonlinear dynamics due to the high angular velocities and perturbations. The SDRE controller is based on cold gas thruster torques to perform the large-angle maneuver in order to reduce the high angular velocities. The main result of this investigation is the approach to numerically approximate the Domain of Attraction.

INTEGRATING MATERIAL SELECTION WITH TOPOLOGY OPTIMIZATION OF MULTI-ALLOY STRUCTURES VIA NEURAL NETWORKS

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ABSTRACT

The design of high performance components such as turbine blades often entails optimizing the geometry as well as selecting the most appropriate alloy(s) for the application. Traditionally, the steps of material selection and geometry optimization are done sequentially, which results in sub-optimal performance. Further, advancements in metal additive manufacturing have enabled the realization of multi-alloy structures, which offer superior performance over single alloy components when the candidate alloys are optimally located.

Towards this end, we propose an integrated approach using variational autoencoders (VAE) and gradient-based optimization methods, to simultaneously select alloys and optimize the topology of parts. In the first step, we consider a database of all candidate alloys described by performance characteristics like yield strength and melting temperature, manufacturing attributes such as feasibility for multi-alloy additive manufacturing, and supply chain attributes such as criticality index. The VAE maps these materials to a continuous, low-dimensional space which can be explored by gradient-based optimization algorithms. This latent space is then coupled with a neural network [1], embedded with a differentiable finite-element solver, to simultaneously optimize the material and topology of the component. Various numerical examples demonstrate the efficacy of the proposed method. Possible extensions to large scale and multi-physics topology optimization are also discussed.

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Theory and application of provably-robust and efficient high-order methods for high-fidelity computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATION OF BOUND-PRESERVING LIMITERS TO THE NONLINEARLY STABLE FLUX RECONSTRUCTION HIGH-ORDER METHOD

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ABSTRACT

The flux reconstruction method has gained popularity in the research community as it recovers promising high-order methods through modally filtered correction fields, such as the Discontinuous Galerkin (DG) method, on unstructured grids over complex geometries. Under a class of energy stable flux reconstruction (ESFR) schemes, the flux reconstruction method allows for larger time-steps than DG while ensuring stability for linear advection on linear elements. For nonlinear problems, split forms and entropy-conserving flux differencing approaches have become popular as they guarantee robustness for unsteady problems on coarse unstructured grids.

Nonlinearly stable flux reconstruction (NSFR) combines the key properties of provable nonlinear stability and the increased time-step from ESFR. NSFR has successfully been applied to unsteady compressible flows in arbitrary curvilinear coordinates with low-storage weight-adjusted approaches to scale efficiently with low memory consumption.

NSFR can also be used in conjunction with bound-preserving limiters to satisfy the maximum principle for scalar conservation laws and preserve positivity in the case of hyperbolic conservation laws. Bound-preserving limiters within an NSFR framework allow for a robust solution to be obtained while preserving the desired properties and maintaining a high-order of accuracy. This study incorporates the implementation of bound-preserving limiters within the NSFR framework to observe the shock capturing capabilities of NSFR. Due to the nature of NSFR and the bound-preserving limiters, solutions for problems involving strong discontinuities are obtained without the use of artificial viscosity or a TVD property while maintaining a high order of accuracy. This study also aims to observe the impact of the flux reconstruction (FR) parameter by implementing the FR parameter adaptively using a shock sensor. The adaptive implementation of the flux reconstruction parameter will allow for more robust solutions. Applying NSFR in the context of shock-capturing encourages the extension of this scheme to a wide range of applications such as compressible turbulence, aeroacoustics, and high Mach number problems. The study is currently performed with preliminary results for 1D and 2D inviscid cases, but the limiter will also be used to extend the NSFR scheme to problems involving complex interactions between viscous shocks, contact waves and viscous boundary layers. The preliminary results include the 1D Sod Shock Tube, Leblanc Shock Tube, Shu-Osher problems as well as the 2D Double Mach Reflection and Mach 3 Wind Tunnel with a Step cases. Results will be provided for the preliminary cases as well as the 2D Daru-Tenaud Viscous Shock Tube case.

Modeling and simulation of coupled processes in geological media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELLING THE FLOW OF FLUIDS THROUGH POROUS SOLIDS EXHIBITING NONLINEAR RESPONSE IN THE SMALL STRAIN REGIME

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ABSTRACT

Considerable experimental evidence in a variety of porous materials (concrete, ceramics, bones, rocks) that undergo infinitesimal deformations makes it clear that material moduli depend on the density (identified as density dependence of Young's modulus).

This is especially relevant for subsurface flows through geological media which have experienced deformation over millenia, and damage or aging manifests in the form of inhomogeneities, and thus density-dependent material moduli.

The fundamental implication of these experiments is the nonlinear mechanical/stress response of the porous solid within the context of “small" deformation. However, the traditional (Biot) theory assumes that mechanical response of porous materials must be linear within the regime of small deformation. Specifically, the porous solid is assumed to be a linearized elastic solid with constant values of material properties such as Young's modulus.

Moreover, incorporating a density-dependent Young's modulus is inconsistent with the assumption of infinitesimal deformation. How can we then have a constitutive theory for porous media that allows nonlinear response within the regime of small deformation ? Furthermore, will the predictions from a nonlinear theory set within the regime of small deformation deviate significantly from that of the (currently used) traditional model ? I propose to definitively answer this question.

Advanced materials: Computational analysis of properties and performance
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INSTABILITY-INDUCED DEFORMATION OF LAYERED CRYSTALS

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ABSTRACT

A family of ternary carbides and nitrides, known as MAX phases, exhibit some of the best attributes of metals and ceramics. Like ceramics, they are lightweight, elastically stiff, thermodynamically stable, and refractory; and like metals, they are damage-tolerant, pseudo-ductile, and machinable. The unique set of properties of MAX phases is generally associated with their layered hexagonal crystal structure, which combines strong intralayer and weak interlayer atomic bonds. Mechanical tests on bulk polycrystalline MAX phases have shown that, unlike their counterpart binary carbides (MX), MAX phases undergo basal slip, cleavage, buckling of layers, and kink-banding. Micromechanical single-crystal level tests have shown that grain-level deformation and failure mechanisms of MAX phases depend on both the crystallographic orientation and deformation constraint of the grains. Building on these recent works, we further analyze the effects of deformation constraints on the mechanical response of single-crystal MAX phases through a series of unconventional small-scale mechanical tests and crystal plasticity finite element analyses. The small-scale tests include three distinct specimen types designed to impose various constraint levels: free-standing micro-pillars, unconstrained micro-walls, and constrained micro-walls. The crystal plasticity finite element analyses employ a non-Schmid crystal plasticity constitutive model, which, based on experimental observations, assumes that the evolution of slip system strength/resistance in MAX phases comprises two components. The first component is the classical element, which depends on the Taylor cumulative shear strain, while the second is the non-Schmid component, which depends on the stress normal to the slip plane. Our primary focus is on understanding the onset of kink-banding, which is essentially an instability. This is motivated by the fact that a few recent experiments have suggested that MAX phases exhibit unconventional damage tolerance because of kink-banding, even in the presence of very weak interlayer bonds. To this end, the focus is confined to a particular crystallographic orientation where the basal planes are parallel to the imposed loading direction. This orientation is the most susceptible orientation for the onset of any instability. Our results show that, regardless of the constraint level, the specimen consistently exhibits susceptibility to the onset of instability. However, the response varies depending on the degree of constraint, with the specimen either undergoing easy cleavage and/or kink-banding. Notably, the crystal plasticity finite element simulations not only replicate the onset of instability in line with experimental results but also approximate the location of these instabilities.

SciML in the real world
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GRAPH CALCULUS NEURAL NETWORK FOR REPRESENTATION OF PHYSICAL SYSTEMS

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ABSTRACT

Universal approximation theorems have advanced the use of Neural networks for parametric interpolation of functions. Among them, Graph neural networks (GNN) are the popular choice for data-driven physics problems for their capability of naturally treating unstructured data. However, many of these physical problems admit to a Partial differential Equation model, desiring the approximation of differential operators in comparison to algebraic functions. The errors in the traditional GNNs due to this limitation are typically mitigated by making the network larger to enrich its representation capacity. The obvious downside of this approach is the inflated demand for training data for these complex networks.

In this talk, we present Graph Calculus Neural Network (GCalcNN) that utilizes a non-local calculus on finite weighted graphs [1] to approximate differential quantities within the network layers. This graph-theoretic framework for modeling builds off on our recent work for representation, exploration, and analysis of computed states of physical systems [2]. We analyze the consistency of the non-local derivatives in this setting, a crucial requirement for numerical applications. We show that the weight of the graph can be fine-tuned to achieve arbitrary order of accuracy in any number of dimensions without any assumptions of symmetry in the underlying data [3]. We first demonstrate the representation capability of GCalcNN for differential operators. Finally, we present three example applications for utilizing this differential representation in learning (1) reduced order models for PDEs, (2) representations for differentiable quantities of interest, and (3) surrogate models for the evolution of PDEs.

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Advanced model order reduction techniques for computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICS INFORMED NEURAL NETWORKS IN THE CONTEXT OF COMPUTATIONAL FLUID DYNAMICS SOLVERS

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ABSTRACT

This contribution focuses on developing a physics-informed neural network (PINN) by incorporating a physics-based loss term derived from an external computational fluid dynamics (CFD) solver, such as OpenFOAM. Building upon our prior research [1], which explored the integration of discretized governing equations with both Artificial Neural Network (ANN) and Long-Short-Term-Memory (LSTM) based neural networks, this work addresses challenges encountered when coupling PINN with external forward solvers.

A significant obstacle in this coupling arises from the difficulty of incorporating the discretized form of the governing equation from the external solver into the computational graph of the PINN. This limitation poses a considerable challenge to the conventional automatic-differentiation-based computation of derivatives for the physics-based loss term concerning the weight matrix and bias vectors in neural networks. To address this, we propose modifying the physics-based loss term to consider the residual generated by the external solver, enabling the computation of the necessary derivatives for the optimization process.

To tackle issues related to high dimensionality, the governing equations are transformed into linear and nonlinear manifolds. The resulting reduced equation form is utilized as a residual for the physics-based loss term in the PINN.

While the advantages of the discretized physics-based neural network are detailed in [1], the primary objective of this work is to integrate available numerical data with established forward solvers for various inverse and ill-posed problems. This approach delegates the tasks of residual computation, handling boundary, and initial conditions to dedicated external forward solvers, such as OpenFOAM, eliminating the need for additional implementation of governing physics within the conventional PINN framework.

Our proposed methods' potential and implementation details are thoroughly examined across several benchmark applications.

Improving the efficiency and accuracy of computational methods through machine learning
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEEP LEARNING-BASED SUPER-RESOLUTION FRAMEWORK FOR HYDRODYNAMIC DOWNSCALING

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ABSTRACT

Understanding fluvial hydrodynamics is crucial for various engineering, hydro-environmental, and geomorphological applications. Physics-based hydrodynamic models predominantly rely on numerically solving the 2D Shallow Flow equations, also known as Saint-Venant equations, derived by depth-integrating the Navier–Stokes equations.
Accurate hydrodynamic simulations depend on high-resolution models, which are prohibitively expensive due to the large temporal and spatial scales involved. On the other hand, low-resolution, computationally affordable models provide only a general perspective of the flow field. In this study, we aim to address this challenge by developing and evaluating physics-aware, deep learning-based super-resolution models. These models generate high-resolution flow fields through downscaling (resolution refinement) of low-resolution, computationally inexpensive, yet inaccurate hydrodynamic simulations. We tested the proposed model across various synthetic and natural domains to identify the strengths and weaknesses of different architectures in different hydrodynamic contexts.

A MIXED NONLINEAR ISOGEOMETRIC PLATE FORMULATION EMPLOYING DUAL BASIS FUNCTIONS

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ABSTRACT

Employing mixed formulations, variables from different fields are discretized independently. Thus, a separate selection of the corresponding interpolation orders is enabled. Determining these independent approximation orders corresponding to the shear-strain equation counteracts shear-locking effects, which occur for standard formulations. In order to improve the accuracy of results further, in isogeometric analysis, non-uniform rational B-splines (NURBS) are selected for the geometry representation and as basis functions that offer a high continuity during analysis. As the additionally introduced parameters increase the computational effort, performing static condensation may be employed to reduce this effect. In nonlinear analysis, this involves determining the inverse of parts of the system matrix in each iteration step of the Newton-Raphson procedure. By selecting dual basis functions for the interpolation of the secondary variables, the relevant matrix part is lumped into a banded matrix with low bandwidth, reducing the complexity of the required matrix inversion. This approach can be employed to increase the efficiency of mixed nonlinear formulations.

In this contribution, the ability of a mixed nonlinear plate element to counteract shear-locking effects and the effectiveness of the proposed condensation procedure in an isogeometric framework are studied for a benchmark example. Therefore, the governing equations for nonlinear plate problems are derived and the shear forces are introduced as additional field. The independent interpolation orders are determined such that they result in matching orders in the shear-strain equation. Furthermore, dual basis functions are employed for the interpolation of the introduced shear parameters, in order to enable an efficient static condensation in nonlinear analysis.

Advanced materials and smart structures: Modeling, simulation and testing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFECT OF LONG-TERM SEA WATER EXPOSURE ON DIELECTRIC MATERIALS

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ABSTRACT

Dielectric materials, which are commonly used in capacitors, could increase energy storage density on a per volume basis in film capacitors compared to current technologies accommodating the ever-increasing power demands. Recent work in this area has brought about dramatic increases in the dielectric permittivity and moderate increases in dielectric loss, leading to increased material performance on a per volume basis. However, little is known about the aging and breakdown of these materials, which could decrease the performance of these films over time due to decaying dielectric loss and energy storage density. A basic study of the aging and breakdown of two different state-of-the-art dielectric materials, 3M's Very High Bond (VHB) 4910, commonly used in actuator applications, and bi-axially oriented polypropylene (BOPP), commonly used in large wound film capacitators, is completed. To begin, accelerated life tests using distilled water are conducted to simulate the aging of these materials in a marine environment. Both cyclic and non-cyclic tensile loading testing are used to characterize the material behavior of the unaged vs aged samples and to determine how the material properties (e.g., tensile strength and viscoelasticity) change over time. For VHB, aging seems to transition the hyperelastic (non-linear) behavior to purely elastic (linear) behavior. In addition, the point of maximum elongation decreases as the amount of aging increases and fracture increases with increasing aging and increasing stretch rate. Elastic modulus also increases with either increasing aging level or increasing stretch rate for VHB 4910. Similar observations can be noted for BOPP, although the effect of its bi-axial orientation must be taken into account. Regardless of stretch rate, decreases in stress and hysteresis are observed as aging time increases. Overall, stretch rate causes an increase in elastic modulus, and the effect of aging looks to be dependent on orientation where for the orientation normal to the long axis, the elastic modulus increases as aging increases and for the orientation parallel to the long axes, the elastic modulus decreases as aging increases. We note that, in every case for BOPP, orientation plays a greater effect on stress and elastic modulus than aging or stretch rate. The success of this work could actively exhibit the promise of these materials in microelectronic uses.

Emerging topology and shape optimization techniques in computational design of materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ACHIEVING PRECISION IN COMPLIANT MECHANISM DESIGN: TOPOLOGY AND SHAPE OPTIMIZATION WITH STRESS AND CURVATURE CONSTRAINTS

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ABSTRACT

Compliant mechanisms (CMs) perform actuation through elastic deformation at flexure hinges. Therefore, precise geometry design of these hinges is crucial for reliable and failure-free operation. Extensive literature has explored the design of CMs, often employing topology optimization. However, applying topology optimization to design flexure hinges presents challenges, primarily due to the absence of an explicit boundary. This difficulty is particularly evident in computational accuracy and determination of the boundary.

In this study, we utilize a sequential topology and shape optimization framework for the CM design [1, 2]. Our focus is on the precise design of flexure hinges through shape optimization in a geometrically nonlinear context. We introduce adaptive shape and domain refinement strategies in the embedding domain discretization method (EDD) to attain both numerically and geometrically accurate designs of the flexure hinges. Additionally, to address the durability and manufacturability of the flexure hinges, we incorporate local stress constraints and a curvature constraint. The design update is implemented by adapting the traction method to the specifics of EDD [3]. Consequently, the curvature constraint is introduced into the auxiliary boundary value problem of the traction method through a penalty functional, instead of being expressed as a response.

As a result, we obtained CMs with smooth and durable flexure hinges due to the presence of stress and curvature constraints. The efficiency and accuracy of the computations were guaranteed with adaptive domain and shape refinements within EDD.

This work introduces the following novelties:

• Extension of shape optimization using EDD to nonlinear elasticity and compliant mechanism design;
• Regularization of the sensitivities via adapted traction method with curvature constraint;
• Adaptive refinement strategies for the computational domain and the embedded shape, tailored for complaint mechanism design.

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Advanced techniques for transport phenomena in heterogenous porous media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HYBRID-SCALE MODELLING AND VERIFICATION OF MICROBIAL MEDIATED REACTIVE PROCESSES IN POROUS MEDIA

Michele Starnoni[*1], Xavier Sanchez-Vila[1], Alberto Guadagnini[2], Monica Riva[2] and Chiara Recalcati[2]*

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ABSTRACT

Simulation of flow, reactive transport, and biomass growth in naturally occurring porous media is of critical importance to several subsurface applications such as CO2 geological storage, oil and gas production and recovery, and groundwater bioremediation. In this talk, we propose a micro-continuum formulation of coupled flow and bio-geochemical reactive transport at the pore-scale, in which the reactive transport model is fully coupled with a biomass-nutrient growth model. The models are implemented into the open-source software BioReactPy. The goal of this talk is twofold. First, we present simulations results of an application case concerning subsurface biomineralization in reactive silicate rocks. Second, we address the important topic of model verification by replicating an experimental setup of calcite dissolution from microscale measurements obtained through atomic force microscopy.

Numerical modelling of composite materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NONLINEAR INTERACTION IN COMPOSITES USING PHYSICS INFORMED NEURAL NETWORKS

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ABSTRACT

Interaction between adjacent constituents within a composite at every scale can be described by nonlinear laws, including unilateral contact and friction that lead to nonsmooth mechanics problems. Numerical evaluation is based on specialized algorithms based on complementarity formulations and nonsmooth optimization, variational and hemivariational inequalities and specialized numerical algorithms which have shown their ability to capture highly nonlinear effects. Alternatively, if one wants to use classical Newton-type algorithms, one may use appropriate penalty functions in order to enforce inequality and complementarity restrictions [1]. Beyond classical numerical approaches, usage of neural networks for calculation of an approximate solution becomes popular, especially within a framework of multiscale finite elements. In the latter case the effect of microstructure, including possible nonlinear interactions, for various loadings is transferred to the homogenized medium through the Representative Volume Element RVE technique. The solution at the RVE level along the iteration steps tolerates some inaccuracies, especially if data-driven constitutive laws are adopted [2]. Usage of physics-informed neural networks, combined with complementarity or penalty formulations for the contact problem is proposed here for the numerical solution of the problem of numerical homogenization including nonlinear interactions at the RVE level. In this context, PINN training [3] can be incorporated at the RVE level in order to provide an approximate solution of the mechanical problem and, subsequently, be integrated within the FE-2 method. Performance comparisons of various alternatives and discussion for further work in the data-driven framework are included.

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Recent advances in numerical methods for mixed-dimensional PDEs
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EVOLVING FINITE ELEMENTS FOR ADVECTION DIFFUSION WITH AN EVOLVING INTERFACE

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ABSTRACT

The aim of this presentation is to introduce a numerical scheme to approximate evolving interface problems for parabolic equations based on the abstract evolving finite element framework proposed by C M Elliott and T Ranner in "A unified theory for continuous-in-time evolving finite element space approximations to partial differential equations in evolving domains" (IMA J. Numer. Anal. 3 (July 2021), 1696–1845). An appropriate weak formulation of the problem is derived for the use of evolving finite elements designed to accommodate for a moving interface. Optimal order error bounds are proved for arbitrary order evolving isoparametric finite elements. The paper concludes with numerical results for a model problem verifying orders of convergence.

Some of the principal contributions of this work are:
- An ALE approach based on evolving isoparametric finite element spaces attached to evolving sub-domains. The evolving mesh is based on moving the Lagrange nodes with a given known smooth velocity. Achieving a higher order method requires a good initial mesh.
- We provide a robust error bound which demonstrates the error in an L_2 norm is bounded, up to a constant, by h^(k+1), where h represents the mesh size and k is the degree of polynomials used both for the discretisation of the domain and the solution. This is the same order error as if we interpolated a known smooth solution.

Methods for identification, machine learning, and uncertainty quantification of reduced order models of coupled systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

OVERVIEW OF THE LATEST FEATURES AND CAPABILITIES OF THE DAKOTA SOFTWARE

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ABSTRACT

The Dakota software package is an open-source and widely used collection of tools for performing uncertainty quantification, optimization, sensitivity analysis, and model calibration on black box computational simulations. Begun as an internal research project at Sandia National Laboratories almost 30 years ago, we estimate it now has thousands of users worldwide in academia, government, and industry. This talk is a brief introduction to and review of Dakota's history and capabilities. Special attention is given to recent developments in algorithms and in Dakota's general usability.

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Emerging frontiers and methods in digital manufacturing: Modeling, simulation, and beyond
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREDICTING RESIDUAL STRESS FIELDS USING A MULTIPHYSICAL MODEL WITH ADAPTIVE REMESHING: MODEL CONSTRUCTION AND VALIDATION

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ABSTRACT

Prediction of residual stresses is critical in the design and analysis of manufactured components. The locations and magnitudes of these fields carries implications for the component strength margins and durability, especially in the presence of notches and flaws.

In this presentation, we construct a multiphysical finite element model to predict the deformed configuration and residual stress fields in a pressure-vessel component resulting from a resistance forge weld in its manufacture. A microstructural constitutive model, BCJ_MEM [1] (adapted from Bammann, Chiesa, and Johnson [2]), is employed to capture microstructural phenomena in the material during the weld process, such as dynamic recrystallization. Adaptive remeshing is employed to ameliorate the significant mesh distortion that results from shear localizations in the Lagrangian finite element model. A mesh convergence study is performed to verify the model predictions and prove mesh insensitivity.

The model construction is complemented by a suite of experimental validation techniques, including physical measurement of displacements and three methods to quantify residual stresses: slitting method, contour method, and neutron diffraction. The model compares favorably to the measurements, and factors that contribute to differences are identified.

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Advances in computational biomechanics and mechanobiology
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AUTOMATED MODEL DISCOVERY FOR PROTEIN MISFOLDING IN ALZHEIMER'S DISEASE

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ABSTRACT

Over the last years, extensive research has supported the tau hypothesis, suggesting that the aggregation and accumulation of hyperphosphorylated tau plays a key role in Alzheimer's disease. However, the intricate dynamics of tau in the human brain remain inadequately understood. To enhance our understanding of the timeline of this process, we discover the best model and parameters to describe the temporal evolution of misfolded tau proteins in different brain regions.

First, based on longitudinal AV1451-PET data from a cohort of n = 162 subjects from the Alzheimer's Disease Neuroimaging Initiative, we create a single heatmap of tau concentrations for all 162 brains across 83 brain regions over the study period varying between three and six years.

Second, we map the data per region into the {c,\dot{c}} space to visualize the characteristic relationship between the concentration of tau and the change in its concentration. In addition, we determine accurate baseline values and carrying capacities per region. This enables us to automatically discover the model and parameters that best describe this relationship across all brains and regions, allowing to quantify the goodness of fit based on data of all subjects.

Third, we partition the entire dataset into Amyloid-β positive and negative status, and explore the effect of amyloid pathology on tau dynamics. We again discover model and parameters for the individual subgroups, systematically comparing the results of these distinct groups. As a result, we create a local, subject-specific model capable of predicting the temporal evolution of misfolded tau proteins in each brain region.

This study not only contributes to advancing our understanding of Alzheimer's disease pathology, but also builds further on a novel approach, integrating a global model with region-specific considerations and automated discovery of the appropriate functions. By linking the specific brain regions to their physiological function, the model enhances the interpretability of Alzheimer's neurodegenerative pathway, allowing for more targeted interventions and personalized treatment strategies in the future.

Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREDICTING EXTRUSION FLOW SHAPES USING DEEP LEARNING

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ABSTRACT

Fluid flow that extrudes through a shaped nozzle can exhibit a different cross-sectional shape than the nozzle itself due to fluid-structure and fluid-fluid interactions after transiting the orifice. These effects have contributed to long-standing problems in manufacturing, particularly in glass/fiber drawing [1], additive manufacturing [2], and microparticle fabrication [3]. Currently, designing nozzles for extrusion flow requires experiments and/or full 3D numerical simulations to determine the extruded fluid flow shape for a given nozzle, which leads to a slow and tedious trial-and-error design process. In this work, a deep learning model based on the U-Net architecture is developed as a standalone solver to predict low-Reynolds number extrusion flow shapes for nested co-axial extrusion flows [3] with remarkable accuracy in a matter of seconds. Although this deep learning model uses full 3D Navier-Stokes simulations for training, once deployed, it completely replaces the computationally intensive tasks of meshing, 3D flow simulation, and streamtracing, enabling rapid design of nozzle geometries and flowrate ratios for desired extrusion flow shapes. The deep learning extrusion flow model developed in this work is validated against both 3D flow simulations and experimental extrusion flow shapes created for bioengineering applications.

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Computational models and methods for predicting cancer progression and treatment response
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MECHANICALLY-COUPLED, BIOLOGY-INFORMED MODELING FOR PREDICTING TRIPLE-NEGATIVE BREAST CANCER RESPONSE TO NEOADJUVANT THERAPY

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ABSTRACT

Neoadjuvant therapy (NAT) is the standard-of-care for treating patients with locally advanced triple-negative breast cancer (TNBC), yet less than half of these patients achieve a pathological complete response (pCR) upon completion of NAT [1]. Thus, it would be highly beneficial to identify early during NAT whether a patient will achieve pCR, as this would enable adapting the treatment to maximize therapeutic outcomes. This study seeks to predict NAT response by improving the mechanical coupling between tumor-induced tissue deformation and tumor dynamics in our previous modeling efforts [2].

We use a reaction-diffusion model to quantify spatiotemporal changes in tumor cellularity as the sum of tumor cell diffusion, proliferation, and death due to NAT. Using two imaging visits (before NAT and after 2 NAT cycles), we calibrate diffusivity, proliferation, and drug efficacy on a patient-specific basis. The model is then run forward in time until a third imaging visit (after 4 NAT cycles) to test predictive accuracy. In [2], the diffusivity was exponentially dampened via the von Mises stress and calibrated globally (i.e., one value per tumor), the proliferation rate was calibrated locally (i.e., one value per voxel in the tumor), and drug efficacy was calibrated globally for each drug. Here, we extend this model to exponentially dampen a globally calibrated proliferation rate via both von Mises and hydrostatic stress to account for compressive stresses within the tumor. Additionally, we locally calibrate the drug efficacy as our sensitivity analysis finds it to be the most sensitive parameter in the model.

We present preliminary results for ten patients comparing predictions from the previous model [2] and the proposed model. When comparing modeled and measured change in total tumor cellularity between the first and the third imaging visit, the concordance correlation coefficients were 0.94 and 0.97 for the previous model and the proposed model, respectively. Thus, our initial investigation into a more comprehensive characterization of mechanical changes during NAT of TNBC showed improved accuracy in tumor cellularity predictions. Future work will aim at further investigating the mechanical coupling on the diffusivity and proliferation rate, adding an advection term, and including an Allee effect in our proliferation term. Then, we plan to construct a model family investigating a subset of these additions and assess the accuracy of various models over the large TNBC dataset.

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THE MECHANICAL SIGNATURE OF REAL AND PLANT-BASED MEAT

Skyler St. Pierre[1], Ethan C. Darwin[1], Divya Adil[1], Magaly C. Aviles[1], Archer Date[1], Reese A. Dunne[1], Yanav Lall[1], Maria Parra Vallecillo[1], Valerie A. Perez Medina[1], Kevin Linka[1], Marc E. Levenston[1] and Ellen Kuhl[1]*

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ABSTRACT

Plant-based meat products have a 50% lower environmental impact than real meat; yet, their adoption into people's diets is globally still low although the market for these products is growing rapidly [1, 2]. The sensory experience, including taste and texture, is rated as one of the most important reasons for choosing which product to eat [2]. Here, we sought to understand the fundamental mechanical properties that characterize real and plant-based based meat products. We tested five plant-based meat products, tofurky, sausage, hotdog, firm and extra firm tofu, and three real meat products, SPAM turkey, hotdog, and sausage, in tension, compression, and shear. In tension, we tested the products until failure, while for compression and shear, we tested to 10% stretch or shear. We found that real meat products tend to have a higher peak stress, but a comparable stretch at peak stress compared to plant-based products. At 10% stretch, real meat products displayed the highest tension/compression asymmetry and were all stiffer in tension than in compression, while some plant-based products were stiffer in compression than tension. We used an 8-term isotropic, incompressible constitutive artificial neural network [3] composed of I_1 and I_2 raised to the power 1 or 2 activated by the identity or exponential function to identity the best constitutive model for each product. Using L_0 regularization, we probed all single- and two-term combinations and collected the mean-squared error of the simultaneous fit to the tension, compression, and shear data. The best models for all meat products included the I_1 term, with all products except firm tofu finding the best fit with two terms. The models for the plant-based products were (I_1, I_2) for tofurky, (I_1, I_2) for sausage, (I_1, I_1^2) for hotdog, (I_1) for firm and (I_1, $\exp(I_1)$) for extra firm tofu. The models for the real meat products were (I_1, I_1^2) for SPAM turkey, (I_1, I_2^2) for hotdog, and (I_1, $\exp(I_1^2)$) for sausage. Two terms, $\exp(I_2)$ and $\exp(I_2^2)$, were never discovered for any products. Understanding the mechanical differences between real and plant-based meat products can guide the design of improved plant-based products to better mimic the mechanical signature of real meat.

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Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CIFEM: ELUCIDATING THE ROLE OF LOCAL THERMAL ENVIRONMENT ON MULTI-TRACK MELT POOL MORPHOLOGY VARIATION FOR INCONEL 718 LASER POWDER BED FUSION

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ABSTRACT

Thermal field prediction of laser powder bed fusion (L-PBF) via physics-based numerical simulation can help optimize the process while avoiding the cost of experimental techniques. However, the widely-used finite element method (FEM) for obtaining layer- and part-scale predictions requires the abstraction of critical physics into an effective heat source model, which invokes a tedious calibration process and provides inaccurate thermal fields compared to computational fluid dynamics (CFD) simulations. Models based on CFD have much higher fidelity but are extremely limited in scale due to the computational expense associated with including relevant physics. Accordingly, the driving force behind multi-track melt pool size variation has remained enigmatic up to this point. In this work, the authors extend the CFD-imposed FEM (CIFEM) to multi-track scenarios for Inconel 718 L-PBF to help address these issues. In this methodology, the thermal fields from the CFD simulation and predicted by a dimensionality reduction-based deep learning framework are imposed on the corresponding FEM solution domain rather than applying any analytically-calculated heat source values. These fields are enforced only within a relatively small computational region encompassing the melt pool, while heat diffusion effects elsewhere are solved via the FEM. To extend to multi-track, CIFEM's data-driven heat source model is trained on multi-track CFD simulations with different scan lengths to establish the role of a local thermal environment metric. The local heat accumulation effect is captured by including this metric: the CIFEM-simulated multi-track thermal fields for different scan lengths possess less than 10% error regarding the high-fidelity CFD simulations, and the simulated melt pool sizes are within 10% error regarding experimental measurements up to five consecutive tracks. The CIFEM model thus provides substantially more accurate thermal process predictions compared to using an effective heat source model and also provides a significant efficiency increase compared to CFD by running on a GPU-based, matrix-free FEM solver that can feasibly be extended to the part scale. These advancements help elucidate the role of local heat accumulation on multi-track melt pool size variation and ultimately can be used to help better identify possible sources of defect formation and improve process-structure-property predictions.

A STUDY ON LOCKING EFFECTS WITHIN THE SOLUTION OF STRUCTURAL MECHANICS PROBLEMS USING PHYSICS INFORMED NEURAL NETWORKS

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ABSTRACT

Key Words: physics informed neural networks, locking effects, collocation

Artificial intelligence (AI) applications have recently gained widespread attention due to their capabilities in the domains of speech and image recognition as well as large language models. This has drawn research attention towards AI and artificial neural networks (ANNs) in particular within numerous branches of applied mathematics and computational mechanics. The challenge of generating extensive training data for supervised learning of ANNs can be addressed by incorporating laws of physics into ANNs. Most of so-called physics informed neural network (PINN) [1] frameworks for structural mechanics applications incorporate the partial differential equations (PDEs) governing a specific problem within the loss function in the form of energy methods or collocation methods.
Many structural mechanics problems are governed by stiff PDEs resulting in locking effects which have already been recognized in the early days of finite element analysis. Locking effects are present for all known discretization schemes, not only for finite elements, independent of the polynomial order or smoothness of the shape functions. This applies to both Galerkin-type solution methods and collocation methods based on the Euler-Lagrange equations of the specific boundary value problem [4].
In this contribution, we examine the impact of stiff PDEs and corresponding locking effects on the accuracy and efficiency of PINN-based solutions of problems in structural mechanics. As a test case, PINN-based solutions of beam problems using shear deformable beam formulations are investigated. Different types of beam formulations are compared with respect to accuracy and efficiency.

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16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Advancements in model reduction, data assimilation, and uncertainty quantification for complex physical systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

REDUCED-ORDER MODELING OF STOCHASTIC CHEMICAL KINETICS UNDER THE LINEAR NOISE APPROXIMATION

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ABSTRACT

Many chemical reaction networks in biology and industrial chemistry involve processes that occur at disparate timescales. This timescale separation permits the systematic reduction of deterministic chemical kinetic models, facilitating parameter estimation and model exploration. In particular, geometric singular perturbation theory provides a coordinate-free framework for deriving reduced mass action models in the deterministic realm. However, for systems of relatively low numbers of molecules, the variance of populations may be important, requiring stochastic models. Interestingly, several studies indicate that timescale separation does not always guarantee the accuracy of reduced stochastic models. In this work, we examine the roles of timescale separation and coordinate transformations in the reduction of the Linear Noise Approximation (LNA) and, unlike previous studies, we do not require the system to be comprised of distinct fast and slow variables. We demonstrate that eigenvalue disparity does not guarantee the accuracy of the reduced LNA. However, through proper coordinate transformation, we are able to recover a reduced model that accurately captures the mean and variance of the LNA. This works demonstrates the need for caution when transferring heuristic model reduction techniques from deterministic problems to stochastic settings.

Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DECA: DISCRETE EVENT INSPIRED CELLULAR AUTOMATA FOR GRAIN STRUCTURE PREDICTION IN ADDITIVE MANUFACTURING

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ABSTRACT

The Cellular automata (CA) approach has been a commonly used method for simulating the microstructure evolution in response to the thermal fields seen in additive manufacturing (AM). The CA approach is computationally cheaper than most other approaches while still maintaining some degree of physical fidelity due to both the decentered octahedral algorithm alongside a calibrated interface response function (IRF). The most common CA approach uses a time-stepped framework which, although it is the easiest to implement while being amenable to parallelization, faces load-balancing challenges when applied to AM problems across multiple compute nodes. This talk introduces a new methodology, inspired by the field of discrete-event simulations, for CA simulations. This new technique, titled DECA, steps in events while also ignoring the global causality constraint (meaning events can happen out of order); however, due to the received events at any cell still following a local causality constraint, the end state of a DECA simulation will still be identical to the end state of a conventional, time-stepped CA simulation (provided the time-step is small enough that the solution is converged). The benefit to using DECA or conventional, time-stepped CA for AM simulations is that it is still relatively easy to implement and amenable to parallelization while also alleviating the load-balancing problem inherent in AM processes (due to the local nature of the process).

Computational geomechanics
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IMPACT OF PARTICLE MORPHOLOGY ON PHYSICAL AND MECHANICAL FEATURES OF GRANULAR MATERIALS VIA DEM INVESTIGATION

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ABSTRACT

Granular materials are commonly encountered in nature, industry, and civil engineering practice, and their mechanical responses are intricately linked to the morphology of the individual particles. As a result, it holds significant theoretical and engineering value to systematically study the inherent connection between the geometric morphology at the particle scale and the macroscopic mechanical behavior characteristics. In this regard, the generation and DEM investigation of physical and mechanical properties of morphological controllable particles are introduced. Firstly, the theories and techniques of geometric reconstruction, and morphological characterization of irregular particles are presented. Secondly, methods for generating virtual particles with controllable multi-level morphological features, including form, angularity and roughness, are introduced. Building upon this, DEM investigations on the particle shape effects on the packing structures and shear behaviors of granular materials are further discussed. The relevant research was financially supported by the National Natural Science Foundation of China (No. 52278364).

Microstructures of chemically complex materials and their impacts on material properties from multiscale simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

UNDERSTANDING THE SOLIDIFICATION AND HEAT TREATMENT CHARACTERISTICS IN THE COCRNISIX MEDIUM-ENTROPY ALLOY BY EXPERIMENTALLY VERIFIABLE MULTISCALE THERMODYNAMIC AND KINETIC COMPUTATIONAL TECHNIQUES

Te-Cheng Su[1], Hao-Chuan Huang[1], Jian-Shiang Chen[1], Jia-Jun Chen[1], Kaifan Lin[1], Hsin-Chih Lin[1] and Jer-Ren Yang[1]*

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ABSTRACT

CoCrNi medium-entropy alloy (MEA) possesses an FCC crystal structure with multiple slip systems and low stacking fault energy [1]; a substantial amount of nanoscale deformation twins can be generated under low-temperature and high-speed deformation. Consequently, this CoCrNi medium-entropy alloy demonstrates exceptional mechanical performance in extreme environments such as space or high-velocity impact scenarios. Adding a proper amount of Si can not only reduce the manufacturing cost and mass density but also enhance ballistic resistance by further lowering the stacking fault energy. Previous studies [2] utilized small-scale vacuum arc remelting techniques to investigate the solid solution or secondary phase strengthening of CoCrNi-based MEAs with Al or Si additions. However, to extend the application of lightweight, high-entropy alloys to industrial-grade impact-resistant plate manufacturing, especially for low-temperature environments, it is necessary to study the solidification and heat treatment characteristics of CoCrNiSix castings. This study employs finite element analysis at the macroscopic scale to investigate the solidification phase transformation and heat transfer characteristics of CoCrNiSix under precision-cast conditions. Additionally, at the mesoscopic scale, the phase-field method [3] is used to simulate the dendritic solidification microstructure and element segregation of CoCrNiSix. Thermodynamic parameters required for simulations are calculated using Thermo-Calc high-entropy alloy databases TCHEA6 and MOBHEA2. This research also utilizes electron microscopy to analyze the microstructures of chemically complex CoCrNiSix ingots, focusing on measuring the secondary dendrite arm spacing and elemental segregation profiles. Collecting these microstructure-related features allows us to reasonably infer the cooling rate corresponding to the precision casting process of CoCrNiSix and design rational parameter combinations for homogenization heat treatment of the cast ingots in terms of temperature and isothermal holding time. By validating macroscopic and mesoscopic simulation results through CoCrNiSix microstructure analysis experiments, the multiscale kinetic computational techniques included in this study can be further applied to cost-saving and process optimization practices in the manufacturing of various lightweight high-entropy alloys.

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Advanced machine learning methods for multiscale modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GRAPH-ENHANCED DEEP MATERIAL NETWORK FOR MULTISCALE MATERIALS WITH MULTIPLE MICROSTRUCTURES

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ABSTRACT

Designing complex multiscale materials requires a comprehensive understanding of their relationships between mechanical behaviors and varying microstructures, leading to extensive research in multiscale materials modeling. In recent years, machine learning methods have emerged as a promising way to accelerate computational multiscale modeling and its time-to-solution predictions of materials behaviors. Among these machine-learning-based multiscale materials modeling methods, the deep material network (DMN) [1] has gained significant attention due to its ability to be used for fast and accurate nonlinear multiscale modeling while only trained on linear elastic data. However, the DMN model can only be confidently used for the specific microstructure it was fitted on, implying that different microstructures need to train other DMN models.

In this work, we adopted a data-driven point of view to tackle the limitation of DMN to a single microstructure. We cleared this roadblock by introducing a graph neural network (GNN) to learn the microscopic informatics of materials through their graph representation. This learned information can be used to generate an appropriate DMN for each microstructure and predict homogenized nonlinear material behaviors. This entire process is integrated under a single umbrella, a hybrid GNN-DMN model. This newly proposed GNN-DMN model [2] can single-handedly treat multiple microstructures and derive their DMN representations for online prediction of structure-property relationships. Examples demonstrate the validity and reliability of the approach, even when it comes to predicting material responses for new microstructures.

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CENTRAL-MOMENT-BASED DISCRETE BOLTZMANN MODELLING OF COMPRESSIBLE REACTIVE FLOWS

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ABSTRACT

Compressible flows, especially the highly compressible reactive flows, have been widely used in modern industry and engineering, for example, in the fields of jet engines and rocket motors. Therefore, understanding compressible reactive flows is crucial to improve the design and performance of modern aircraft, rockets, engines, and other advanced technologies. In fact, the compressible reactive flows generally encompass a wide variety of nonlinear, unsteady, and nonequilibrium processes. Besides, both hydrodynamic and thermodynamic nonequilibrium influences are usually prominent, and the range of timescales involves several orders of magnitude. To probe the dynamic process, a central-moment-based discrete Boltzmann model (CDBM) is developed for highly compressible reactive flows. Via the Chapman-Enskog analysis, the CDBM is demonstrated to recover the Navier-Stokes (NS) equations in the hydrodynamic limit. Moreover, it provides quantification of thermodynamic nonequilibrium effects beyond the NS equations. The capability of the CDBM is demonstrated through simulations of the sound wave, thermal Couette flow, sod shock tube, shock reflection, and detonation wave. It should be mentioned that, compared with the previous discrete Boltzmann models, the CDBM can provide the nonequilibrium effects of highly compressible reactive flows which related to the thermal fluctuation directly. This work is helpful to have a better understanding of highly compressible reactive flows, and provide reliable numerical data for further improving the technologies of aeronautics and astronautics, energy and power engineering.

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STUDY OF FAILURE EVOLUTION IN SHOCKED POROUS SOLIDS BY COMPARING MATERIAL POINT METHOD AND MOLECULAR DYNAMICS SIMULATIONS

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ABSTRACT

Understanding the failure evolution in porous solids (or architected materials) under impact loading has become an important research topic over the past decade because their well-designed porous structures can result in high energy dissipation to weight ratios as compared with non-porous solids. Especially, multiscale failure evolution in shocked porous solids plays an important role in optimizing blast/impact-resistant design scenarios. Material Point Method (MPM) and molecular dynamics (MD) share significant similarity in the sense that both are particle methods. The MPM is a continuum-based particle method that displays great potential in simulating large deformation and multi-phase interaction problems beyond the nanoscale. The MD is a discrete particle method in which an appropriate potential function is utilized to calculate the interatomic forces and to describe the motion of an atomic or molecular system. However, it is still a challenging task to validate MD responses against the experimental data due to the spatial and temporal limitations in impact and/or shock tests. Therefore, this study mainly aims to conduct a series of impact simulations of porous solids by using the MPM and MD to understand the differences and similarities between these two spatial discretization approaches. Since both MD potential function and MPM constitutive modeling are well-formulated for metallic solids, we establish a computational model with 40 nm×40 nm×40 nm porous and non-porous gold cubic targets impacted by full density non-porous gold cubic flyers with an extreme high speed for the comparative study. The overall deformation patterns and particle-velocity histories are analyzed and illustrated with the use of the two particle methods. It appears that the MPM and MD can capture consistent physical responses, which shows the potential of using the MPM for multiscale simulations of extreme events with available verification and validation capabilities.

Imaging and computational methods for biomechanics
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FROM MEDICAL IMAGE TO COMPUTATIONAL DOMAIN: METHODOLOGY AND APPLICATIONS

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ABSTRACT

This study introduces a robust pipeline for converting medical images into computational domains, addressing a significant gap in the current integration of these images into computational simulation frameworks. Standard medical image formats, such as those from computed tomography (CT), are not inherently structured for direct application in computational simulations. Thus, preprocessing is essential to delineate shapes and interfaces within the Region Of Interest (ROI), enabling an accurate computational representation of the physical domain.

The proposed methodology is crucial in computational biomechanics, where medical images serve as a primary source for simulating various physical phenomena, providing the necessary geometric foundation. The transition from CT scans and similar modalities to operational computational domains is complex, especially with open-source tools.
Common commercial software, like Avizo from ThermoFisher Scientific, often involves subjective choices impacting the reliability of computational domains. Our methodology offers a systematic approach for the automatic preprocessing of structures and microstructures (from micro-CT), ensuring high-fidelity representations while maintaining resolutions compatible with the capabilities of contemporary computer simulation technologies in terms of memory and computational time.

To demonstrate the applicability of such a methodology, two example cases are considered : i) the analysis of a porous microstructure obtained from a human meniscus sample, and ii) the analysis of a multi-body system considering the digitization of a tumor embedded inside a human brain. In both cases, the entire computational process is considered, from the medical image to the simulation and post-processing of the results to verify the reliability of the computed discretized domains, either tetrahedral distributions for finite element (FEM) applications or point clouds representation for the discretization corrected particle strength exchange method (DC-PSE)

Mesh-free particle methods for multi-physics problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADAPTIVE COUPLING OF BULK AND THIN FILM FLOW MODELS USING MESHFREE METHODS

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ABSTRACT

Various thin film flow models have been proposed in literature to study the flow of fluids in thin layers. These models have been widely used when the thin fluid film is only object of interest. However, these models are not applicable when a bulk flowing fluid hits a curved surface and forms a thin layer of fluid over it. Such scenarios commonly occur, for example, in cleaning processes in the food industry. Simulations of such flow typically rely on bulk (3D) fluid models, with excessively fine resolutions in the thin flow regions, which make them prohibitively expensive.

In this talk, we present a novel adaptive fluid modelling framework to simulate coupled bulk-surface fluid flow. The proposed framework uses a traditional 3D Navier--Stokes model for bulk fluid flow, and switches to a pseudo 2D thin film flow model when appropriate. The bulk and thin film flow both involve free surfaces and can undergo significant deformations. Thus, the bulk fluid and thin film fluid layers are both modelled using meshfree methods. Thus, this forms a meshfree-meshfree coupling.

The framework proposed automatically identifies regions where the thin film model is applicable, and adaptively changes the fluid model used. In this talk, we will discuss how the models are coupled, and how mass conservation is ensured when switching between the two meshless models. Numerical results are verified against fine bulk simulations, and applications to cleaning simulations in the food industry, and automotive water crossing simulations are presented.

New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A STRUCTURAL TOPOLOGY OPTIMIZATION METHOD USING PHYSICS-INFORMED NEURAL NETWORKS BASED-ON KL EXPANSION

Koutarou Suetake[*1], Kazuhiro Izui[1], Kozo Furuta[1] and Shinji Nishiwaki[1]*

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ABSTRACT

Topology optimization is a widely utilized method in engineering design for optimizing the material distribution within a given design domain to achieve optimal performance under specified constraints. In recent years, Physics-Informed Neural Networks (PINNs) have emerged as a noteworthy alternative to the Finite Element Analysis (FEA) conventionally employed in topology optimization. However, with the increase in the number of parameters in a neural network, there is a corresponding rise in computational requirements.
The approach of topology optimization using Karhunen-Loève (KL) expansion, as proposed by Y. Tsukuda, K. Furuta, K. Izui, S. Nishiwaki, and S. Watanabe [1], stands out for significantly reducing the number of parameters. This reduction serves to effectively mitigate the associated computational costs. This study proposes a novel approach to topology optimization integrating PINNs and KL expansion. The method comprises a neural network representing the displacement field and a neural network representing the density field. The displacement field is solved using a PINN introduced in [2], employing a Fourier Features neural network architecture with boundary conditions implemented as hard constraints. The neural network for the density field using KL expansion can learn weights by the loss gradient in the neural network for the displacement field. Applying KL expansion to the density field neural network has result in a substantial reduction in design variables has been achieved.

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Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DIFFUSIVE-DISCRETE CRACK TRANSITION SCHEME REALIZED BY EXTENDED B-SPLINE-BASED IMPLICIT MATERIAL POINT METHOD

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ABSTRACT

A novel procedure is proposed to realize transition from a diffusive crack to discrete crack topology within the framework of the extended B-spline-based implicit material point method (EBSMPM) [1]. After the formulation is explained in detail, the specific manner of how the EBS basis functions are constructed is explained. At the end, several representative numerical examples, one of which includes a large rotation problem, are presented to demonstrate the performance of the proposed method.

The crack initiation and propagation are determined by the crack phase-field model, and the damage distribution is obtained as the diffusive crack that is continuously distributed in the body. Based on the damage distribution, we determine the location of the discrete crack surface and generate a new physical boundary to represent separation of the body. Specifically, on the basis of the idea that the damage gradients are supposed to be normal to the potential crack surface, the discrete crack surface is identified as the location where the damage gradients are inverted [2]. Once the location of the discrete crack surface is identified, the transition from the diffusive crack to discrete crack is performed by applying the extended B-spline (EBS) basis functions [3]. To date, in the mesh-based methods and even in the MPM, additional degrees of freedom (DOFs) and remeshing are required to represent the strong discontinuity. On the other hand, in the proposed transition scheme, the EBS basis functions are constructed so that the support domain of the basis function contains only a single physical domain separated by the discrete crack surface, which is the novel concept presented in our study. Thus, the proposed scheme does not need the additional DOFs and remeshing with reconfiguration of connectivity and reconstruction of tangent stiffness matrices.

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Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CRACK PROPAGATION SIMULATION USING DAMAGE MODEL AND FINITE COVER METHOD

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ABSTRACT

In this work, we examined the crack propagation simulation using the finite cover method regardless of the mesh. The present method uses a damage model to estimate the initial crack and crack propagation. Recently, multi-material structures have been widely used in many engineering fields; thus, crack propagation simulation needs to estimate crossing different types of materials, such as steel and plastics. In particular, the adhesion area between different materials is important to predict the structural behavior that affects the accuracy of the products. In previous work, the authors have presented the crack propagation simulation using a damage model for ductile fracture. Ductile failure is one of the unsolved problems in computational mechanics. The continuum damage mechanics has been developed for predicting material behavior. These assume that the microscopic voids govern the ductile failures and that their mechanisms consist of a few major steps. In this work, we adopt this concept to deal with the crack propagation simulation for multi-materials. The so-called damage parameters are major state variables, and their evolution laws are the main interests in these mathematical models. However, these models can clearly describe the discontinuities because these modeling approaches treat the ductile fracture as a parameter, and the discontinuities describe immersed boundaries. On the other hand, we focus on the simulation methods. The conventional finite element simulation(FEM) is not good at handling the discontinuities, especially in crack propagation analysis because the FEM describes the discontinuities by themselves elements boundaries. Moreover, generalized finite element methods have been developed mainly in fracture mechanics. The extended finite element method(X-FEM) is well-known for simulating crack propagation, mainly in linear elastic bodies. This method can easily simulate the nucleation and growth of discontinuities (cracks) by the character of enhanced approximation function.
By contrast, the finite cover method(FCM)is also proposed as one of the generalized finite element methods. The FCM can describe the discontinuities by multiple covers, which is based on the concept of this method. Consequently, some numerical examples show that FCM with the damage model simulates the crack propagation for simple multi-material structures.

Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PRACTICALITY INVESTIGATION OF THREE-DIMENSIONAL LIMIT EQUILIBRIUM METHODS FOR WIDE-AREA LANDSLIDE PREDICTION

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ABSTRACT

For wide-area landslide risk assessment, numerous approaches have been proposed, but most rely on statistical or simple physics-based models. To elevate the landslide risk assessment with reasonable accuracy and reliability, the advanced physics-based models should be examined for practical applications.

This study investigates the performance and practicality of a variety of the 3D Limit Equilibrium Methods (LEMs) based models by comparing their results with actual landslide events. Specifically, the Hovland method [1], 3D simplified Bishop method [2], and 3D simplified Janbu method [2] are targeted. These methods compute normal and shear forces on soil column surfaces using local equilibrium equations, then integrate them into global equilibrium equations for moment, vertical force, or horizontal force equilibrium equations to determine the factor of safety.

To discuss the accuracy of each method, a comprehensive slope stability analysis targeting Marumori Town, Miyagi, Japan, where numerous slope failures resulted from heavy rainfall induced by Typhoon Hagibis in 2019, is conducted for the comparative study. Both the geological maps and borehole data repositories determine the soil parameters used in the analyses. Considering the landslides during intense rainfall are typically shallow, the slip surface depth is constrained between 0.5 to 5.0 meters in the iterative calculations.

Using a factor of safety threshold value of 1.0, the True Skill Statistics (TSS) revealed a tendency of the Hovland method to overestimate the hazardous areas relative to the other methods. In contrast, Area Under the Curve (AUC) results suggested a consistent level of accuracy across all methods when no specific threshold was imposed. In other words, the Hovland method can yield similar hazardous areas and TSS values to other methods by employing different factor of safety thresholds. Thus, while variations exist in the calculated factor of safety, it is confirmed that the Hovland method can produce results comparable to more advanced methods by adjusting the factor of safety threshold.

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Quantum scientific computing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

QUANTUM ANNEALING FOR STRUCTURAL DESIGN

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ABSTRACT

Abstract
Solving optimization problems using quantum computing has recently received significant attention due to its advantages in quantum mechanics and the extensive development of quantum machines. One promising algorithm is known as quantum annealing [1], building upon the simulated annealing algorithm used in classical computers. However, quantum annealing exploits the quantum tunneling effect to accelerate the search for the optimal solution, enabling it to outperform in various aspects, especially in the speed of searching for the solution [1, 2]. To date, quantum annealing has been applied in various applications, demonstrating its robust performance [3]. However, based on existing literature, only a few studies have investigated the use of quantum annealing for structural optimization. In fact, a unified structural design framework using quantum annealing, applicable to both truss and continuum structures, has yet to be developed.

In this study, a structural design framework has been developed from the perspective of using quantum annealing as one of the heuristic optimizers. A hybrid approach is adopted, utilizing a classical computer for structural analysis and quantum annealing for topology updating as gradient-free topology optimization. The minimization of the compliance problem with a volume constraint is selected as the objective function and then transformed into a quadratic unconstrained binary optimization (QUBO) format, incorporating the penalty method and slack variable for the constraint. In addition, the encoding process for the design variable is implemented and then updated in each design iteration. To demonstrate its performance, the developed method is applied to the design of both truss and continuum structures. The results indicate that the proposed framework demonstrates promising performance in converging to an optimal topology.

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Data-driven approaches for solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SOLVING PARTIAL DIFFERENTIAL EQUATIONS WITH PHYSICS-INFORMED NEURAL NETWORKS BASED ON A DUAL VARIATIONAL PRINCIPLE

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ABSTRACT

In recent work [1], an approach to devise a variational principle for linear and nonlinear PDEs such as Navier--Stokes equations, nonlinear elasticity, and time-dependent heat equation was proposed. In [1], the essential idea is to treat the primal PDE as a constraint and to invoke an arbitrarily chosen (lends flexibility) auxiliary potential with strong convexity properties to be optimized. This leads to requiring a convex dual functional to be minimized subject to Dirichlet boundary conditions on dual variables, with the guarantee that even PDEs that do not possess a variational structure (in primal form) can be solved via a variational principle.

In this presentation, we explore a new route to solve PDEs that require the imposition of Dirichlet and/or Neumann conditions in physics-informed neural networks (PINNs) [2]. To this end, we adopt ideas from [1] to tackle linear and nonlinear problems using PINNs. In standard PINNs [2], different terms that meet boundary conditions have to be weighted as loss terms in the objective function, which adversely affects training of deep neural networks and the accuracy that it can deliver. Improvements such as using approximate distance fields to impose Dirichlet boundary conditions have been proposed [3], but further advances are needed. Herein, we leverage the dual variational principle, which provides greater flexibility---since the Dirichlet boundary conditions on dual variables can be arbitrarily chosen. The parametric dependence of the dual solution on the choice of Dirichlet boundary conditions (and the auxiliary potential) appears to offer practical advantages in training and optimization of neural networks, and the fact that the dual-to-primal map always yields the unique primal solution, when such uniqueness is a property of the primal problem. To illustrate this new approach, we assess the use of the dual variational principle on several boundary-value problems in heat conduction and solid mechanics, and compare its performance to standard PINNs.

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Quantum scientific computing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

QUANTUM SOLVER OF STOCHASTIC DIFFERENTIAL EQUATIONS

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ABSTRACT

Stochastic differential equations (SDEs) model the random behaviors of systems and can be applied in various fields such as natural sciences, engineering, and finances. In many cases, SDEs do not have analytical solutions, and the numerical solving process requires exhaustive Monte Carlo sampling, which is computationally expensive. Recently, quantum computing arises as a new paradigm for scientific computing [1,2]. In this work, we propose a new approach to simulate the stochastic dynamics of SDEs on quantum computers. The stochastic behavior is embedded into quantum states. Probability distributions are encoded with computational basis. The proposed approach is demonstrated with several SDE examples. To verify the accuracy, the simulated results are compared with the classical Monte Carlo simulation. The statistical moments are compared quantitatively.

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Geomechanics of the cryosphere
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SEA ICE MODELING IN DOE'S ENERGY EXASCALE EARTH SYSTEM MODEL (E3SM)

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ABSTRACT

We provide an overview and describe progress for the MPAS-SI-MPM project [https://mpas-si-mpm.unm.edu]. The purpose of MPAS-SI-MPM is to enhance the representation of sea-ice mechanics in DOE's Energy Exascale Earth System Model (E3SM) using an elastic-decohesive constitutive model for the ice. The ultimate goal is improving coupled climate simulations and predictions. The more descriptive physics contained in the constitutive model provides a mechanism to model leads explicitly, and to account for frazil ice and dense water formation in leads, for example. The improved representation is expected to generate more realistic coupling fluxes to the atmosphere and ocean.

The model is implemented using the material-point method (MPM). MPM provides a Lagrangian representation of sea ice which allows transport of state variables and tracers without numerical diffusion, as well as history along trajectories for constitutive models. Platform portable GPU acceleration is achieved through the polyMPO library which supports material point operations on spherical centroidal Voronoi tessellation/unstructured meshes and is built using the Kokkos library and the PUMIPic library from the SciDAC FASTMath Institute. To assess model performance, techniques for parameter calibration and model validation (especially for leads) are being developed. These techniques depend on new metrics for analyzing spatiotemporal data with discontinuities, and/or lower dimensional features.

SELF-STABILIZED 3D VIRTUAL ELEMENTS FOR LINEAR ELASTOSTATICS: HU-WASHIZU VARIATIONAL FORMULATION FOR POLYHEDRA WITH LINEAR TRIANGULAR FACES

Dexin Sun[1], Elias Pescialli[2], Massimiliano Cremonesi[2], Umberto Perego[2], Alessandro Russo[34], Carlo Lovadina[54] and Qun Li[1]*

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ABSTRACT

Abstract
The traditional finite element method (FEM) is severely limited by the quality of the elements and highly distorted or concave elements are not allowed. The Virtual Element Method (VEM), originally proposed by Beirão da Veiga et al. [1], can be viewed as a development of the traditional FEM. The VEM does not require isoparametric mapping and does not exhibit distortion sensitivity, so it is very flexible and versatile, allowing for arbitrary polyhedral meshes, not necessarily convex. However, the stiffness matrix of the virtual element requires stabilization in most cases [2], which is one of the main limitations of the VEM. This paper proposes a new type of 3D self-stabilized virtual elements, without needing a stabilization process, based on a Hu-Washizu variational approach for 3D linear elastostatics [3]. Since the external surface of this new 3D element is composed of an arbitrary number of triangles looking like the capital Delta (Δ), we named it Deltahedron element. The advantage of triangles over faces of arbitrary polygonal shapes is that the displacement model on a triangular face is completely defined by nodal values. The numerical tests conducted on these Deltahedral elements, including non-convex shapes, showed good accuracy and the expected convergence rate. Deltahedral virtual elements can be effectively used to discretize 3D structures, including those with curved surfaces.

Keywords: Virtual element method; Self-stabilized Virtual Elements; Deltahedral elements; Hu-Washizu variational approach; 3D linear elastostatics

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Advances and applications of polytopal methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HYDRAULIC FRACTURE SIMULATION OF MESO-CONCRETE USING THE SBFEM-FVM MODEL

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ABSTRACT

This paper explores the simulation of the coupled interaction between mesoscale crack water pressure and the process of mesoscopic crack initiation and propagation in concrete, treating it as a three-phase material consisting of aggregates, mortar, and interfaces. A hybrid approach, combining the scaled boundary finite element method (SBFEM) and finite volume method (FVM), is employed at the microscale to model the interplay between crack water pressure and mesoscopic crack evolution. The cohesive crack model is applied to analyze the non-linear fracture transition zone. When multiphase materials are present within the crack tip element, the crack propagation direction is determined by generalized stress intensity factors and the fracture toughness of each phase material. Comparisons of numerical results with experimental data reveal a close correspondence between F-CMOD curves and water pressure variations under different loading conditions. The impact of crack water pressure on the mesoscopic concrete crack propagation direction is emphasized. This coupled model provides valuable insights into the interrelation of mesoscale phenomena and macroscopic behavior in brittle concrete materials. The findings contribute to an enhanced understanding of fracture processes in concrete structures, particularly under varying environmental and loading conditions.

Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MPM LAGRANGIAN-EULERIAN HYDROCODE FOR SIMULATING BURIED EXPLOSIONS IN TRANSVERSELY ISOTROPIC GEOMATERIALS

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ABSTRACT

Shock waves in geological materials are characterized by a sudden release of rapidly expanding gas, liquid, and solid particles. These shock waves may occur due to explosive volcanic eruptions or be artificially triggered. In fact, underground explosions have often been used as an engineering solution for large-scale excavation, stimulating oil and gas recovery, creating cavities for underground waste storage, and even extinguishing gas field fires. As such, hydrocodes capable of simulating the rapid and significant deformation under extreme conditions can be a valuable tool for ensuring the safety of the explosions. Nevertheless, as most of the hydrocodes are often formulated in an Eulerian grid, this setting makes it non-trivial to track the deformation configuration of the materials without a level set. The objective of this presentation is to propose the use of the material point method equipped with appropriate equation of state (EOS) models as a hydrocode suitable to simulate underground explosions of transverse isotropic geomaterials. To capture the anisotropic effect of the common layered soil deposits, we introduce a new MPM hydrocode where an anisotropic version of the Mie-Gruneisen EOS is coupled with a frictional Drucker-Prager plasticity model to replicate the high-strain-rate constitutive responses of soil. By leveraging the Lagrangian nature of material points to capture the historical dependence and the Eulerian calculation of internal force, the resultant model is capable of simulating the rapid evolution of geometry of the soil as well as the high-strain-rate soil mechanics of anisotropic materials.

Recent developments in peridynamics modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SUPERPOSITION-BASED CONCURRENT MULTISCALE APPROACHES FOR PORODYNAMICS

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ABSTRACT

Superposition-based concurrent multiscale approaches for porodynamics problems aimed at resolving localized fluid flow and deformation of a solid skeleton including its possible fracture or strain localization are developed. The main departure of the proposed formulation is that the primary unknowns in the coupling zone, the solid displacement u and pore pressure p, are discretized by possibly different numerical models. Two discretization schemes are studied: (i) superposition of two or more finite element (FE) discretizations of the Biot's u-p model of a porous medium, and (ii) superposition of the peridynamics (PD) discretization of the fractured solid phase on the FE discretization of the Biot's u-p model of a porous medium. In the latter case, the total stress of the fluid–solid mixture in the coupling domain is derived from the effective stress obtained from the combined PD and finite element method solutions while the pore pressure is obtained from the FE solution. The accuracy of the superposition-based concurrent multiscale method is studied on several benchmark problems including the classical Terzaghi's one-dimensional dynamic consolidation problem, the two-dimensional strip footing dynamic problem, the sand liquefaction induced strain localization and the fluid-driven fracture propagation problem in saturated porous media. The main strain localization phenonmenon and hydraulic fracture characteristics have been found to be reasonably well reproduced by the proposed method.

Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SEISMIC DAMAGE ANALYSIS OF UNDERGROUND FRAME STRUCTURES WITH PERIDYNAMICS

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ABSTRACT

Strong earthquake poses a significant threat to the structural integrity of underground frame structures. This paper presents an innovative seismic damage analysis method for underground frame structures based on superposition-based coupling of Peridynamics (PD) and Finite Element Method (FEM). In the numerical model, peridynamics (PD) is employed to simulate underground structures, effectively capturing the initiation and propagation of cracks within the structures, while the surrounding soil is simulated using FEM. The efficacy of the proposed numerical methods is assessed through comparison with dynamic centrifuge tests. The nonlinear collapse and failure mechanism of the Daikai Subway station during the 1995 Kobe earthquake are elucidated. Numerical results demonstrate that this approach facilitates the replication of damage patterns in underground frame structures subjected to seismic effects, with an explicit representation of cracks. A parametric study is conducted to explore the influence of key factors on the damage patterns of underground frame structures.

MODELING AND SIMULATION OF HYDROGEN-DEFECT INTERACTIONS IN NANOSTRUCTURED METALLIC MATERIALS ACROSS MULTIPLE TIME SCALES

Xingsheng Sun[*1]*

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ABSTRACT

Hydrogen (H), the lightest and most abundant element in the universe, plays a pivotal role in shaping the future landscape of energy and sustainability. Its significance lies in its extraordinary versatility as an energy carrier, capable of efficiently storing and transporting energy derived from diverse sources. However, as H-based energy systems become more prevalent, material challenges associated with H detection, storage, and transport remain a bottleneck to be addressed. For example, crystalline defects such as dislocations and grain boundaries are commonly found in metallic materials. Therefore, the interactions between H atoms and lattice defects are of paramount importance, as they profoundly influence the mechanical, electrical, and chemical properties of materials. In this talk, we will employ two numerical methods to unravel H-defect interactions in nanostructured metals across multiple time scales. The first method, referred to as Diffusive Molecular Dynamics (DMD), focuses on capturing hydride phase transformation and the evolution of H-induced lattice defects over a diffusive time scale. The second method, Molecular Dynamics (MD), provides more detailed insights into atomic movements and lattice relaxation over the time scale of thermal vibrations. These two methods are connected with MD simulations initialized using statistical measures of microscopic variables obtained from DMD at different H concentrations. Our focus will be on the palladium-hydrogen (Pd-H) systems. Our study demonstrates that DMD can effectively capture the H diffusion mechanisms over an extended time scale as well as the dynamics of solute-induced misfit dislocations and stacking faults. While the H-concentrated phase leads to a reduction in the vibrational energy, the presence of stacking faults locally increases the vibrational energy of both Pd and H atoms. Furthermore, the MD simulation results align with DMD in terms of equilibrium potential energy, the preservation of hydride phase boundary, and the spatial distribution of stacking faults. We thoroughly characterize the lattice crystalline structures in four key regions of the particle. We observe a preference for H atoms to occupy tetrahedral interstitial sites near stacking faults due to the lower stacking fault energies provided by these sites within the H-concentrated phase.

Modeling mechanics of materials with voids
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PORE EFFECTS ON THE PROPERTIES OF TRIPLY PERIODIC MINIMAL SURFACE BONE SCAFFOLDS

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ABSTRACT

As an important strategy in the field of bone tissue engineering to deal with necrosis of the femoral head, the triply periodic minimal surface bone scaffold has become a promising candidate for bone repair due to its excellent structural properties, including excellent mechanical properties, biocompatibility, and promotion of tissue regeneration. A strong candidate that has received much attention in the field. In this context, the pore structure plays a crucial role in the construction of triply periodic minimal surface bone scaffolds. How to properly select and regulate the properties of triply periodic minimal surface bone scaffolds to make them compatible with the repair of the target bone area The matching of requirements has become a problem that needs to be solved urgently. The purpose of this review is to summarize the significant impact of pore structure on the properties of triply periodic minimal surface bone scaffolds, and to provide guidance and inspiration for the development and manufacture of such bone scaffolds. In the process, the effects of factors such as pore shape, porosity, pore size, curvature, and specific surface area on the properties of triply periodic minimal surface bone scaffolds were briefly outlined and discussed, in order to provide useful reference for future research and practice.

TRANSLATING BIOLOGY TO ENGINEERING THROUGH MULTIPHYSICS COMPUTATIONAL MECHANICS

Adamya Singh Dhaker[1], Yuchen Sun[1], Francesco Regazzoni[2], Luca Dede'[2], Cecilia Laschi[1] and Gianmarco Mengaldo[1]*

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ABSTRACT

Life's key to survive in nature is the smart adaptation to its complex surrounding environments. Cephalopods muscular hydrostats, which consist only of muscle tissues and preserve volume during deformation, are a well-known example of biological entities which exhibit infinite degree-of-freedom motion and manipulation to perform complex environment-oriented tasks. One such muscular hydrostat of interest is the octopus arm, which has exceptional flexibility and dexterity to achieve complex motion. Several experimental studies from a biological and neuromuscular control perspective, as well as soft-bodied robotics perspective have been conducted to understand and exploit octopus morphology, which lacks a rigid skeleton, for a multitude of engineering applications. However, there are very few computational simulation frameworks which accurately model and capture the precise activation sequences and resultant motion in octopus arms. Here, we present a high-fidelity, 3-D computational model of octopus arm biomechanics, replete with muscular fiber arrangements and muscle activation strategies which mirror those of a biological counterpart (Octopus vulgaris). An octopus arm geometry is modelled in the multiphysics solver life-x, with a
biologically similar implementation of longitudinal and transversal muscle fibers. The material properties of the arm follow the Neo-Hookean constitutive law, with an isovolumetric constraint applied to the geometry and Dirichlet, Robin and Neumann boundary conditions at the base, curved surface and tip respectively to mimic a fixed arm immersed in a fluid environment. Three primary movements shown by octopus arms are elongation or shortening, bending and reaching. All three movements are elicited through different activation profiles on the same muscle fiber segments by applying stresses which follow the sequential nature of muscle activation found in real octopus. The most characteristic octopus arm motion is the reaching motion, which involves the propagation of a bend from the base to the tip in order for the octopus to grasp an object. Our model is able to mimic and capture the biomechanics of the reaching motion with significant accuracy. The analysis shows that the simulated bend follows the same fundamental kinematic profiles for displacement and bendpoint tangential velocity, which are invariant across specimen, as physical experiments. The simulation framework provides a biologically accurate platform for creating digital twins of biological entities, which can be leveraged to extract valuable physics as a benchmark to the field of modeling and fabrication in soft robotics community.

Imaging-based methods in computational medicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMAGE-BASED VASCULAR FLUID-STRUCTURE INTERACTION WITH ANISOTROPIC FIBER-REINFORCED ARTERIAL WALL MODELS

Yujie Sun[*1], Ju Liu[1], Jiayi Huang[1], Qingshuang Lu[1], Xinhai Yue[1] and Xuanming Huang[1]*

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ABSTRACT

In this study, we present a computational framework for vascular fluid-structure interaction (FSI), which enables image-based geometric modeling for anisotropic arterial walls. This framework employs the unified continuum formulation for monolithic FSI coupling [1]. In particular, the variational multiscale formulation is invoked to handle the incompressibility constraint. The arterial walls are constructed using segmentation techniques as well as physiological knowledge of the arterial wall thickness. The modeling of the multi-layer arterial walls can be conveniently realized through the same vein. The Holzapfel-Gasser-Ogden (HGO) constitutive material model is employed here for the arterial walls. This material model features the exponential form of the strain energy and takes fiber dispersion into account. It characterizes the mechanical behavior of vascular tissues to high accuracy. Furthermore, we also develop a technology for fiber direction definition of the arterial wall model. It leverages the vascular centerline to define the local basis, which can be conveniently utilized to determine fiber direction at each quadrature point.

The developed fiber generation method is evaluated by comparing with a strategy from a previous study [2]. It is shown that our approach yields satisfactory fiber definitions in patient-specific models. Additionally, through two numerical examples, we investigate the impact of anisotropic arterial wall models on the vascular FSI. The first case involves a simulation of an idealized curved geometry, and the second case investigates an image-based abdominal aorta model. The numerical results reveal that under physiologically realistic conditions, the transmural stress distribution within anisotropic arterial walls is significantly different from that of isotropic models. Lastly, we consider a two-layer model for the abdominal aorta, and each layer is treated as the HGO model with different fiber orientations and material parameters. Compared to the single-layer model, significant differences are again observed in a variety of biomechanical quantities of interest. Our work suggests that the arterial wall model has a non-negligible impact on the computational modeling of vascular problems.

Keywords: Anisotropic, Multi-layer, Vascular fluid-structure

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Multiscale, multifield, and continuum-discontinuum analysis in geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NONLOCAL MANIFOLD FRACTURE MODEL FOR MULTIFIELD-DISCOTINUOUS PROBLEMS IN GEOMECHANICS

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ABSTRACT

Multifield-discontinuous problems play a pivotal role in geomechanics, where understanding and predicting crack propagation in geomaterials under multiphysical fields, such as fluid flow and heat transfer, is essential for practical guidance. This study focuses on the development of a novel nonlocal model that quantitatively describes the continuous-discontinuous deformation of geomaterials and its interaction with fluid and heat fields in a unified and objectively geometric manner.

Our model involves the formulation of nonlocal momentum balance laws for a continuum manifold. The resulting governing equations are established within the fiber bundles of the continuum manifold, emphasizing the intrinsic geometric characteristics of discontinuous deformation. This geometric approach renders the model suitable for constructing nonlocal transport equations for fluid and heat when voids and cracks appear in geomaterials.

Theoretical and computational results demonstrate that our proposed model is asymptotically compatible with classical continuum mechanics as the characteristic length of the nonlocal interaction domain approaches zero. This study underscores the significance of nonlocal and geometric characteristics in describing the balance laws of discontinuous deformation in geomaterials involving multifields. Our findings are validated through comparisons with experimental data and existing theoretical models, showcasing the accuracy and applicability of the proposed model.

This study significantly contributes to the comprehension of continuous-discontinuous deformation in geomaterials under multiphysical fields. The insights gained can provide valuable guidance for optimizing productivity in real-world applications.

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OPTIMIZATION METHOD OF FIBER REINFORCED PLASTIC (FRP) COMPOSITE STRUCTURES

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ABSTRACT

Fiber reinforced plastic (FRP) composite structures are made from fiber fabrics or tapes. Tape-laying and overwrapping process, by which the fiber angle and thickness would change with the radius of structure, are two common manufacturing methods for the FRP composite structures. Therefore, the curvature radius and geometry are coupled with fiber plying parameters during the optimized design of the FRP composite structures. In this study, Moving Morphable Components (MMC) method, which is able to explicitly describe the geometry of structures, is used to perform topology optimization for FRP composite sandwich and stiffiened structures. The FRP composite structures are considered to be manufactured based on geodesic winding, with fiber plying angle and thickness calculated according to the curvature radius of each beam. The stiffness and deformation of FRP composite structures are then analyzed by Finite Element Method. The numerical and experimental results indicate the validity of the proposed optimization method.

Transport phenomena in micro/nanofluids
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PARTICLE DYNAMICS IN A LOW-REYNOLDS-NUMBER FLUID BETWEEN TWO SPHERICAL SHELLS

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ABSTRACT

Dynamics of a particle and the suspending low-Reynolds-number fluid confined between two spherical shells were studied numerically. We calculated the particle's hydrodynamic mobilities at various locations in the confined space. The mobility is largest near the middle of confined space along radial direction and decays as the particle becomes closer to no-slip walls. Fluid vortices in the confined space induced by the particle motion were observed and analyzed. We also found that the particle can exhibit a drift motion perpendicular to the external force. Magnitude of the drift velocity normalized by the velocity along the direction of the external force depends on particle location and particle-to-cavity sizes ratio. This work forms the basis to understand more complex dynamics in microfluidic applications such as intracellular transport and encapsulation technologies.

AN IMMERSED BOUNDARY MMALE PARTICLE METHOD FOR EFFICIENT MODELING FSI PROBLEMS WITH STRUCTURAL DAMAGE

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ABSTRACT

Fluid-structure-interaction (FSI) phenomena with multi-phase flow dynamics and structural damage commonly exist in engineering practice, which however bring great challenges to nowadays numerical FSI algorithms. A novel localized subdomain smoothing MMALE particle method (ls-ALEPM) is proposed in this paper for efficient and accurate simulations of large scale FSI problems. The MMALE method and the MPM are strongly coupled by immersing the MPM particles into the MMALE grid. In order to avoid the spurious strain induced by the mixed FSI velocity field, a decoupled stress updating scheme is proposed to update the stress of solid particles by introducing a virtual velocity field in the vicinity of FSI interface. And specifically, the highly accurate polyhedron intersection based method is employed for its remapping phase, which however is time-consuming. Thus, the localized subdomain smoothing method (LSSM) is put forward to accelerate the remapping phase which only involves the distorted regions of computational grid. The LSSM is composed of a distorted subdomain determination step and a combinated mesh smoothing step. Each iteration of the combinated mesh smoothing step consists of the modified GETMe and the weighted average method, and the transfinite interpolation method is adopted if the quality criteria is still not satisfied after prescribed maximum number of iterations. The validity and efficiency of ls-ALEPM is verified by several benchmark numerical examples and practical engineering simulations.

Fluid dynamics and SciML: Navigating challenges and seizing opportunities
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TACKLING TEMPORAL DOMAIN COMPLEXITY TO EFFECTIVELY TRAIN PINNS FOR UNSTEADY FLOWS PAST MOVING BODIES

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ABSTRACT

Physics-informed neural networks are a class of neural networks that embed physics-based constraints into the loss function, proving viable for solving inverse problems when data is limited. Recently, for unsteady flows past moving bodies, motivated by the benefits of PINNs and the immersed boundary method, an immersed boundary-aware (IBA) surrogate modeling framework has been proposed[1]. This framework removes the limitations of case-specific computational domain transformations to the body-attached frame of reference. Under this framework, two variants of PINN models have been proposed, one suitable for scenarios where body position and velocity are known apriori and another for scenarios where those need to be estimated along with the flow-field variables.

In either setting, one might encounter temporal domain complexities in terms of temporal sparsity, a large temporal domain, or rich spectral content in the flow field data. The present study explores temporal domain decomposition strategies[2] to tackle such scenarios. Assuming the body position and velocity are known, the moving boundary-enabled PINN (MB-PINN) variant under the IBA framework is chosen for velocity flow-field reconstruction and pressure recovery. Specifically, the sequential and backward-compatible extensions of MB-PINN are explored for temporal domain decomposition. Flow past a plunging elliptic airfoil at a low Reynolds number is considered an example.

For a periodic flow case, when velocity data snapshots are temporally sparse, a backward-compatible version performs better than standard MB-PINN in both pressure recovery and velocity reconstruction. Moreover, this version only requires a single network at inference. However, in the case of a large time domain, where, breaking the temporal domain into relatively smaller segments is necessary to reduce problem complexity, having multiple small sub-networks is beneficial to avoid training large networks. Currently, it is also being investigated if these sequential training methods are beneficial when the flow-field data has richer spectral content in the temporal domain as in the case of flow-field aperiodicity.

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Biomechanics of hard tissues: From experiments and simulations to clinical applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A COMPARATIVE STUDY OF DIFFUSION-BASED AND RATE-FORM MODELS IN BONE REMODELLING

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ABSTRACT

Dynamic evolution of cells, viz. osteoclasts and osteoblasts, is pivotal to bone remodelling. The present study comprehensively compares diffusion-based models and phenomenological rate forms that predict the dynamic evolution of osteoblasts and osteoclasts. Primarily, our work focuses on the influence of messenger substances with the aim of decrypting the intricate mechanisms governing the evolution of these cells, shedding light on dominant timescales affecting their progression. Diffusion-based models in our study account for the complex inter-connected processes governing remodelling and include a) osteocyte evolution mediated by flexoelectric signalling [1] as opposed to models depending on mechanical stimuli [2], b) coupled diffusion equations with cell evolution dependent on messenger substance evolution unlike other works in literature, c) accounting for anisotropic diffusivity under thermodynamic constraints, and d) accommodating osteocyte apoptosis, a critical precursor to osteoclast and osteoblast evolution [3]. We demonstrate the numerical implementation of diffusion-based and phenomenological models within the Finite Element framework and highlight the advantages of coupled diffusion-based approaches. In addition, we also validate the coupled diffusion-based models with clinical data to emphasise the sensitivity of various parameters to cellular mechanotransduction and anisotropic growth.

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Machine learning and multiscale modeling for complex materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DESIGNING ARCHITECTED MATERIALS USING NEURAL NETWORKS

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ABSTRACT

Design of architected materials, i.e., microstructural optimization, is a special case of topology optimization where the objective is to find the optimal distribution of material within a representative unit cell, to result in a desired homogenized behavior. A popular strategy for designing architected materials, i.e., microstructures, is the density field method where a pseudo-density field is defined and optimized over an underlying mesh to achieve a desired objective. Typically, the density field is represented using an underlying finite element mesh.

In this talk, we propose a neural network (NN) framework where the density field is represented using the NN's activation functions, weights, and biases. The decoupling (1) avoids manual sensitivity analysis derivation through automatic differentiation, (2) prevents checkerboard patterns without additional filters, (3) supports recovery of high-resolution microstructural topology via a simple post-processing step, and (4) supports easy extension to multiple materials.

In the proposed framework, any of the microstructural quantities, namely, bulk, shear, Poisson ratio, or volume, can serve as the objective, while the remaining can be subject to constraints. The framework is illustrated through a variety of microstructural optimization problems.

Quantum scientific computing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN IMPROVED BOX ALGORITHM FOR SOLVING LINEAR SYSTEMS OF EQUATIONS ON QUANTUM-ANNEALING MACHINES

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ABSTRACT

A typical strategy for solving linear systems of equations on quantum annealing machines is to pose them as quadratic unconstrained binary optimization (QUBO) problems. The underlying principle is to represent the unknowns (i.e., real numbers) in a radix-2 qubit form and iteratively converge to the desired solution by minimizing the underlying potential energy. The box algorithm [1] is a robust iterative implementation of this strategy.

However, the box algorithm suffers from two main problems. Firstly, it faces convergence issues when the potential energy is relatively flat. Secondly, it fails to recycle the computed solution in successive iterations.

In this talk, we will present an improved box algorithm that addresses both these deficiencies. This is illustrated through several numerical experiments. We then apply the improved box algorithm to compute sparse approximate preconditioners for large matrices, arising from partial differential equations [2].

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Contact and interface mechanics: Modeling and computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RATE-DEPENDENT ADHESION AND SUCTION EFFECTS IN CONTACT MODELING OF POROELASTIC MATERIALS USING FINITE ELEMENT METHOD

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ABSTRACT

The demand for poroelastic soft materials in biomedical and engineering applications is increasing exponentially due to their remarkable resemblance to biological soft tissues and unique mechanical properties. The study of mechanical responses of poroelastic soft material under contact scenarios is one of the active areas of research which is essential for reliable performance of the parts made with these materials. The characteristics of poroelastic multiphasic soft swollen materials rely on the behavior of the solid matrix and the interstitial fluid. Soft multiphasic materials undergo large deformations and exhibit mechanical response that is both dependent on the rate of deformation and characterized by nonlinearity. However, the existing computational models often overlook the influence of adhesion in the contact formulation, neglecting its significance in representing real-world scenarios. The purpose of this study is to bridge this gap by incorporating the rate-dependent adhesion effects for poroelastic material contact into an open-source nonlinear finite element analysis code FEBio.

Indentation is a commonly used technique to identify the dependency of contact phenomenon on a broad range of loading and unloading rate, relaxation time, and coupling of adhesion and friction. The main obstacle of contact formulations is to precisely determine the active contact zone within the interface by solving a constrained optimization problem with an appropriate set of Karush-Kuhn-Tucker (KKT) conditions. This research aims to explore the mechanics of rate-dependent adhesion and the associated suction effect within a poroelastic contact model. Our primary objective is the modification of the FEBio source code to incorporate effective traction-based contact formulation with nuanced intricacies of adhesion at interface. In addition, the comprehensive capture of rate-dependent adhesion characteristics is focused on the identification of the active contact zone through the KKT condition. The simulation results following the compilation of the modified source code are validated against experimental results. The adaptation of the FEBio source code to include a rate-dependent adhesion, coupled with the precise determination of the active contact zone through the KKT condition, not only sets out to enrich our understanding of material behavior but also improves the capabilities of computational tools towards more authentic simulations of intricate biological interactions.

Fluid dynamics and SciML: Navigating challenges and seizing opportunities
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATION OF AUTOENCODER-BASED DEEP OPERATOR NETWORK (DEEPONET) TO PRODUCTION-SCALE CHEMICALLY REACTING COMPUTATIONAL FLUID DYNAMICS SIMULATIONS

Bryan Susi[*1], Somdatta Goswami[2], Ameya Jagtap[3], Hessam Babaee[4] and George Karniadakis[3]*

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ABSTRACT

Integration of numerically stiff chemical reaction systems is a challenging problem that can significantly restrict the temporal scale of achievable Computational Fluid Dynamics (CFD) simulations of chemically reacting flows. Sufficiently resolved integration of stiff chemical systems reduces the allowable timestep of a CFD simulation such that even massive parallelization of the spatial domain cannot enable tractable simulations as the temporal evolution is not as efficiently aided by distributed domain parallelization. Other mitigation strategies like using unconditionally stable solvers for the chemical systems, tabulation procedures, or reduced-order kinetics models have been used successfully, but each approach manifests different inaccuracies that affects CFD simulation credibility. We present recent work of applying Deep Operator Networks (DeepONet) with an Autoencoder-Decoder framework to learn the temporal evolution of stiff chemical systems within the context of a CFD simulation. The purpose is to investigate an alternative approach to conventional mitigation methods employed by CFD practitioners. Recently published results [1] have demonstrated that an autoencoder-based DeepONet can predict temporal evolution of a stiff ordinary differential equation system with acceptable accuracy while relegating the costly temporal integration to offline training. This is particularly suitable for CFD simulations because a single learned model with more complex chemical kinetics can support many simulations without as much cost for in-situ chemical source term evaluation, and with improved chemical species evolution. The presented method does not address sub-grid scale localization of reactions, nor turbulent mixing; therefore, error is invariably introduced during the presented DeepONet approach. The motivation of this presented work is to investigate whether the access to greater temporal range and more complex reaction mechanisms is advantageous for select applications relative to the impact of incurred error.

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Advances in damage & fracture modeling of multiphysics materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LEVERAGING A NEURAL NETWORK-ENHANCED REPRODUCING KERNEL PARTICLE METHOD FOR MULTIPHYSICS DEGRADATION MODELING OF ENERGY STORAGE MATERIALS

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ABSTRACT

Energy storage materials exhibit strong electro-chemo-mechanical coupling and highly anisotropic material properties, contributing to the formation and propagation of micro-cracking during charge/discharge cycling and resulting in reduced performance and service life. A coupled electro-chemo-mechanical reproducing kernel particle method (RKPM) formulation has been developed to analyze this system. With microstructural images supplied by the National Renewable Energy Laboratory (NREL), pixel-based model construction by RKPM is used to represent the complex material microstructures that dictate the coupled physics of these systems. Traditional electro-chemo-mechanical models rely on mesh-based finite element methods, which can lead to difficulties in meshing such complex geometries and capturing crack propagation due to mesh dependency. Here, a neural network-enhanced reproducing kernel particle method (NN-RKPM) [1, 2] is introduced to effectively model damage and crack propagation in the material microstructures; the location, orientation, and solution transition near a localization are automatically captured by superimposed block-level NN optimizations. This NN enrichment approach allows for effective modeling of localizations via a fixed background discretization, relieving tedious efforts for adaptive refinement in traditional mesh-based methods. Applications to the heterogeneous microstructures of Li-ion battery cathodes will be presented to demonstrate the effectiveness of the proposed methods. NN-RKPM is additionally used to inform how crack opening and closure in turn affect the coupled chemical equations and material microstructure.

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Recent advances in partitioning method and interface mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FRACTURE SIMULATION OF FEMTOSECOND LASER-INDUCED DAMAGE IN MULTI-LAYER DIELECTRIC COATINGS

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ABSTRACT

We present a dynamic fracture simulation to study the femtosecond laser-induced damage in multi-layer optical coatings. We modeled the formation and propagation of cracks in an expanded hafnia layer in a blister created through laser-induced damage using finite element analysis. The extended finite element method (XFEM) is used to simulate the propagating crack. We validate our mechanical modeling and crack propagation with experimental results supported by X-TEM measurements.

Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EVALUATION OF MECHANICAL PROPERTIES OF THREE-DIMENSIONAL POLYCRYSTALLINE MICROSTRUCTURES OF DUAL-PHASE STEEL USING MACHINE LEARNING MODEL BASED ON PHASE-FIELD METHOD AND CRYSTAL PLASTICITY FINITE ELEMENT METHOD

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ABSTRACT

In this study, mechanical properties of three-dimensional polycrystalline microstructures of dual-phase (DP) steel are evaluated using a machine learning model. DP steel is composed of a soft phase (ferrite) and a hard phase (martensite). The mechanical properties of DP steel depend on the spatial distribution of martensite, which contributes to strength, and ferrite, which contributes to ductility.

In the material development of DP steel, there is a need to improve the trade-off relationship between strength and ductility. However, material development requires repeated experiments through trial and error. To reduce experimental costs, numerical simulations are used. The crystal plasticity finite element method (CPFEM) is used to take the effect of crystal orientation and grains size into account. However, CPFEM is computationally expensive, especially in three-dimensional analysis. Therefore, convolutional neural network (CNN) is utilized to replace CPFEM in this study.
Microstructures of DP steel are generated in two steps in this study. For the first step, polycrystalline microstructures are generated using the multi-phase-field method. The multi-phase-field method predicts whether each grid point is within a crystal grain or grain boundary. Next, the results of the multi-phase-field method are used as initial states of the phase-field method that predicts martensitic transformation. By extracting the results before martensitic transformation has fully developed, microstructures with various volume fraction of martensite can be obtained.
CPFEM is used to evaluate the mechanical properties. Using CPFEM, the stress-strain relationship for each microstructure is obtained. We employ the maximum stress and the working limit strain obtained from the stress-strain relationship as mechanical properties. The maximum stress is the indicator for strength, and the working limit strain is the indicator for ductility, respectively.
CNN is trained by setting the DP steel microstructure generated by the multi-phase-field method and the phase-field method as input, and the maximum stress and the working limit strain as output. By replacing CPFEM with the trained CNN, a framework is constructed to rapidly repeat the generation of DP steel microstructures and the evaluation of the mechanical properties of the generated microstructures. Using the framework, the effects of grain size and the volume fraction of martensitic phase on strength and ductility in three-dimensional polycrystalline microstructures of DP steel are evaluated.

Applications of shape optimization in complex engineering problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPLICIT FEATURE SIZE CONTROL IN PARAMETER-FREE SHAPE OPTIMIZATION

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ABSTRACT

Parameter-free shape optimization [1] is a powerful tool for designing structures when an exact boundary description is required. This technique, arguably a misnomer, directly parameterizes nodal coordinates of a finite element mesh, allowing a design to be optimized directly from a nonlinear programming solver. The lack of a mesh-independent parameterization allows great design flexibility; however, feature size control remains a challenge. Namely, limiting the smallest allowable feature of an optimized design is almost always required in practice, but is a non-trivial constraint to enforce in parameter-free shape optimization.

Here we present a differentiable constraint that enables explicit feature size control, allowing users to set minimum feature sizes in optimized designs. The constraint works by computing the distance between relevant boundary integration points and computing a smooth minimum of these distances. Determining which boundary integration point distances are relevant for computing a feature size is a focus of this research. Further, the constraint formulation is used to compute both positive and negative features of a design, which a user may wish to limit depending on the manufacturing process utilized. Feature size control is demonstrated using this constraint on both 2D and 3D shape optimization problems.

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Large-scale structural and fluidic topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MACHINE LEARNING APPROACH FOR TOPOLOGY OPTIMIZATION OF SELF-SUPPORTING STRUCTURES USING GRAPH NEURAL NETWORKS

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ABSTRACT

Additive manufacturing (AM), also known as 3D printing, has revolutionized the landscape of manufacturing, offering unprecedented design freedom and customization capabilities. Unlike traditional subtractive manufacturing methods, which involve cutting away material from a solid block, additive manufacturing builds objects layer by layer from digital designs. This layer-by-layer approach enables the fabrication of highly complex geometries with intricate internal structures. In tandem with this technological leap, the significance of topology optimization has surged. Topology optimization aims to determine the optimal distribution of material to achieve desired performance objectives while satisfying various constraints. Traditionally employed in engineering disciplines such as aerospace, automotive, and mechanical engineering, it minimizes weight, maximizes stiffness, or enhances other performance metrics of structural components. The synergy between topology optimization and AM presents a compelling opportunity to push the boundaries of design and manufacturing, offering novel designs unattainable with conventional manufacturing techniques.

As the demand for optimized designs continues to grow, the challenge of computational expense in topology optimization remains a significant hurdle to overcome. The intricate nature of topology optimization problems, with their vast array of design variables and iterative optimization processes, often requires substantial computational resources. Machine learning approaches can be used as a tool to expedite the topology optimization process. In this paper, we use a graph neural network to propose a framework specifically for the topology optimization of overhang-free parts. In this paper, we propose a framework specifically for the topology optimization of overhang-free parts using a graph neural network. Eliminating overhangs is crucial because they require support structures, which are laborious to remove and add to manufacturing costs. Our approach integrates automatic differentiation (AD), streamlining sensitivity analysis and reducing computational overhead. This method enhances computational efficiency and facilitates the seamless integration of sensitivity analysis into the optimization pipeline, addressing both 2D and 3D problems under mechanical and thermomechanical loading. By leveraging AD, our framework eliminates the need for explicitly coding sensitivity calculations, enabling efficient optimization even with complex overhang filters.

Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LARGE DEFORMATION MESHFREE ANALYSIS USING HIGHER-ORDER GRADIENT CRYSTAL PLASTICITY

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ABSTRACT

Mechanical behavior of metallic materials is strongly influenced by the size effect at the micrometer scale. The conventional crystal plasticity theories, which are widely used for the meso-scale modeling of polycrystalline metals, do not represent the size effect because these theories cannot consider the accumulation of dislocations. Therefore, the higher-order gradient crystal plasticity models have been proposed for taking the dislocation information into account to describe the size effect. In this model, geometrically necessary dislocations (GND) are introduced into a hardening function of the slip system. In this model, the following governing equations for displacement and GND density fields should be simultaneously solved.
The finite element method, which is the most popular method to solve a problem in the solid mechanics, sometimes provides an improper solution in the higher-order gradient crystal plasticity analysis. Therefore, the development of a numerical method to solve the higher-order gradient plasticity is essential. In this study, the reproducing kernel particle method (RKPM), which is a kind of meshfree method, is introduced into the higher-order gradient crystal plasticity analysis. In order to improve the accuracy and stability of the analysis, the stabilized conforming nodal integration is adopted as the numerical integration scheme. Several numerical examples are demonstrated, and an advantage of the RKPM for solving the large deformation problem with the higher-order gradient plasticity model is discussed.

Innovations in machine learning-enhanced uncertainty quantification for computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE MODELING AND SIMULATION PLATFORM FOR PREDICTING COLD DWELL FATIGUE IN TI ALLOYS

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ABSTRACT

Failure due to fatigue is a key concern in the aerospace industry. While plasticity in general is understood to govern failure in aerospace-grade titanium alloys, various experimental and modeling studies over the past few decades have revealed the role of the underlying microstructure in controlling plastic deformation and subsequent failure. Numerous multiscale modeling approaches have evolved to delineate the role of these key factors. The development of a continuum-scale plasticity framework that can model plasticity at structural length scales while explicitly accounting for the microstructural features and predicting fatigue crack nucleation has posed a consistent challenge to the modeling community. This work discusses the development of a unique class of novel modeling approach referred to as Parametrically Upscaled Constitutive Models (PUCM) and Parametrically Upscaled Crack Nucleation Models (PUCNM) framework for prediction of structural-scale fatigue crack nucleation in α/β Ti-6Al-4V alloys, whose polycrystalline microstructures contain micro-texture regions (MTRs). This approach provides a thermodynamically consistent upscaled constitutive framework to bridge spatial scales through the explicit representation of microstructural descriptors in the constitutive equations in the form of Representative Aggregated Microstructural Parameters (RAMPs). The coefficients of model parameters in the PUCM are functions of the RAMPs. The fatigue life of a specimen has shown strong dependence on the presence of MTRs. A novel MTR intensity measure is formulated in this work to quantify the effect of its presence. This is incorporated in the PUCNM framework as a RAMP. A database of probability of crack nucleation and the corresponding RAMPs are developed using the Crystal Plasticity Finite Element (CPFE) model [1]. Using this database, a functional form of the macroscopic indicator for crack nucleation probability (R) is identified using Genetic Programming based symbolic regression (GPSR). The capabilities of the PUCM/PUCNM are demonstrated by simulating two different types of specimens, a structural scale compressor disk from an aircraft engine, and a Double Edge Notched Tensile (DENT) coupon specimen. The microstructural features represented by RAMPS obtained from EBSD micrographs are distributed on these specimens while preserving the spatial correlation based on 2-point statistics. This location-specific distribution of RAMPs allows the investigation of the effect of microstructural as well as geometric features on crack nucleation. Uncertainty in the fatigue life due to variability in microstructure is also quantified this way.

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Large-scale structural and fluidic topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MICRO-SCALE TOPOLOGY OPTIMIZATION FOR THERMAL-FLUID PROBLEMS USING FTT-BASED HOMOGENIZATION METHOD

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ABSTRACT

The demand for miniaturization and higher performance in electronic devices continues to increase. Consequently, the increase in the heat generation density inside electronic devices has made thermal countermeasures even more challenging. Therefore, research and development of new cooling technologies to maintain electronic devices at appropriate temperatures is being actively pursued. For example, porous metal materials and micro lattice structures have been proposed as heat dissipating structures. These structures with fine voids are expected to increase the heat transfer area between solids and fluids and improve the cooling performance. However, narrow flow paths increase flow resistance. In other words, there is a trade-off between pressure loss and cooling performance, making satisfactory design difficult. Furthermore, theoretical methods to design such materials or structures do not exist yet.

In this study, topology optimization based on the homogenization method is developed as a microstructure design method for heat exchange structures. Topology optimization based on the homogenization method is an effective method for designing materials and structures with hierarchical or multi-scale structures. The characteristic feature of the homogenization method is the separation of the governing equations into a micro boundary value problem and a homogeneous (average) governing equation. In this study, the Stokes equations and the heat advection and diffusion equations are assumed as the governing equations on the micro scale.

To solve the micro boundary value problem, the Fast Fourier Transform (FFT)-based homogenization method is utilized. Conventionally, the finite element method (FEM) is used as a numerical analysis method for homogenization problems. On the other hand, the FFT-based homogenization method has been proposed as a more efficient method than FEM for solving homogenization problems [1].

The proposed method is applied to the maximum heat transfer coefficient problem and the results are discussed.

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Multiscale modeling, analysis and numerical methods of material defect and inhomogeneities
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DISLOCATION DYNAMICS ANALYSIS OF BASAL PLANE DISLOCATION NEAR THE SURFACE IN 4H-SIC

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ABSTRACT

4H-SiC has recently become a focus of attention as a new power semiconductor material that could replace silicon. One of the challenges for its practical application is the reduction of basal plane dislocations (BPD) in the epitaxial layer. In devices utilizing SiC, it is known that device performance deteriorates due to the expansion of stacking faults that accompany the movement of BPD [1]. BPD typically dissociates into partial dislocations, which exist as pairs of 30°-30° and 30°-90° partial dislocations based on the angle made between the dislocation line and the Burgers vector. During the growth of the epitaxial layer, almost 30°-30° partial dislocation pairs are converted to threading edge dislocations [2], but the conversion mechanism has not been clear yet. On the other hand, 30°-90° partial dislocation pairs do not remain in the epitaxial layer [3], and the reason is not clear. Therefore, it is essential to elucidate the behavior of BPD partial dislocation pairs. Molecular dynamics analyses have been conducted, but an interatomic potential that accurately reproduces dislocations near surfaces has not yet been developed.
In this study, 2D dislocation dynamics analysis was performed to clarify the behavior of BPD partial dislocation pairs near the surface of 4H-SiC. Based on the dislocation theory, the forces acting on the dislocation were calculated by the stress field around the dislocation near the surface obtained by the finite element method (FEM), and the equilibrium distance between two partial dislocations was calculated. The results indicated that the equilibrium distance of BPD partial dislocation pairs decreases as they approach the surface. Meanwhile, the translational force exerted on the dislocation pairs was found to be inactive for the 30°-30° partial dislocation pairs, whereas it significantly increased for the 30°-90° partial dislocation pairs as they approached the surface. This result suggests that a potential explanation for the exclusive persistence of 30°-30° partial dislocation pairs within the epitaxial layer. This result suggests that only 30°-30° partial dislocation pairs remain in the epitaxial layer.

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Boundary element methods: New theories and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A BOUNDARY-INTEGRAL-EQUATIONS-FRIENDLY SHAPE OPTIMISATION FOR PERFECTLY ELECTRIC CONDUCTORS

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ABSTRACT

This study establishes an adjoint-variable-method-based shape optimization for 3D electromagnetic scattering problems regarding PECs. The main contributions of this study are to derive (i) the new expression of the shape derivative on the basis of the surface current density, which is usually solved with boundary integral equations (e.g. EFIE, MFIE, CFIE) and (ii) the explicit form of the EFIE and MFIE for the adjoint problem. Some numerical examples verify the correctness and applicability of the proposed shape optimisation.

Multiphysics and data-driven modeling for cardiovascular biomedicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE POTENTIAL OF UTILIZING OPENSOURCE SOFTWARE FOR ESTIMATING HEMODYNAMIC PARAMETERS OF THE AORTA

Ryo Takeda[*1], Katsuhiko Sasaki[1], Shinya Honda[1], Hiroichi Yokoyama[2], Nobuyuki Oshima[1], Akiyoshi Kuroda[1], Hideyoshi Takashima[3], Chenyu Li[3], Hiroaki Date[1] and Hiroyuki Kamiya[2]*

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ABSTRACT

Aortic dissections and ruptures are the most fatal conditions of aortic aneurysms which is said to have caused over 170,000 deaths around the world in 2019[1]. This work aims to present the potential of utilizing an opensource software (OSS) based platform as clinical tool for risk assessment of acute aortic dissections and ruptures. First, three-dimensional surface aorta models are created from chest CT DICOM image files of patients. Image segmentation is implemented through active contours and thresholding of CT values. Then, CAD is used to construct the analysis model which consists of the ascending(AAo) and descending aorta(DAo) as the inlet and outlet respectively. Boundary conditions mimicking a human pulsation[2] was applied to these inlet and outlets by flow pressure and flowrate. The aortas used in this work were classified into three different types: healthy (no dissection or aneurysms), Stanford type A (dissection at AAo) and Stanford type-B (dissection at DAo). Finally, an OSS OpenFOAM was used to calculate the pressure distribution, flow velocity and wall shear stress (WSS) within the three different types of aorta models. The simulation method showed that points of high WSS, concentrated in the areas where the aorta was torn into the true and false lumen. This indicated that these areas are at high risk being damaged from pulsatile flow from the heart. Therefore, the proposed OSS platform has the potential of locating high risk rupture areas that could assist in selecting proper treatment methods in the clinical field.

16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Advances in discretization techniques, element technology, mesh adaptivity, and solution strategies for inelasticity, localization, and failure

July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADJOINT SENSITIVITY ANALYSIS AND DESIGN OPTIMIZATION FOR LAGRANGIAN SHOCK HYDRODYNAMICS

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ABSTRACT

Numerical methods for the Euler equations of compressible fluid flow are widely used in the study of shock physics. While these methods yield predictions of the flow given fixed problem parameters, one often additionally desires sensitivities of these solutions to the problem parameters, say to enable design optimization or for inverse identification of unmeasurable experimental conditions. This talk describes a discrete adjoint method for efficiently computing sensitivities in shock hydrodynamics problems. For the discretization, we use a Lagrangian-description, high-order finite element method, which has been shown to confer several advantages, such as exact mass conservation, perfect resolution of material interfaces, and amenability to efficient implementation on modern supercomputer architectures [1,2]. Time integration is accomplished with high-order explicit finite difference schemes, and shocks are captured with a suitable artificial viscosity approach.

We discuss the formulation and implementation of the discrete transient adjoint (that is, the “discretize-then-differentiate” approach) [3], including appropriate smoothing of the discrete problem to ensure differentiability, and the judicious use of automatic differentiation tools to simultaneously obtain ease of implementation and good computational efficiency. Finally, we demonstrate the method with highly nonlinear design optimization problems inspired by inertial confinement fusion research and illustrate its potential to help advance this field.

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Machine learning algorithms for accelerating material characterization, discovery, design, and manufacturing processes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICS-INFORMED MACHINE LEARNING OF THE THERMODYNAMICS AND KINETICS OF POINT DEFECTS IN ALLOYS

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ABSTRACT

Desirable properties of multi-component alloys, such as corrosion, high-temperature oxidation and irradiation resistance, are highly sensitive to the formation and migration of point defects such as vacancies and interstitials. Point defect formation, diffusion and the associated energy barriers are governed by the interactions between individual and/or groups of atoms. In this work, we use Machine learning (ML) algorithms in tandem with molecular dynamics based Nudged Elastic Band (NEB) calculations to learn the composition- and configuration-dependent formation energies and migration barriers for vacancies. Specifically, we train deep neural network models using numerical representations of the local configurational environment and also implement a physics-informed approach ensuring that the detailed balance criteria are obeyed. We discuss various scenarios including i) comparison of results using relaxed as well as unrelaxed geometries, ii) multiple methods to implement the detailed balance criteria and iii) compositional complexity by comparing vacancy energetics in Cu-Ni and Cu-Au and Fe-Co-Ni_Ti alloys and iv) configurational complexity by comparing vacancy and interstitial defects in Cu-Ni.

Recent advances in computational fracture mechanics and failure analysis
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HOW TO USE STATISTICAL FRACTOGRAPHY AND COMPUTATIONAL FRACTURE MECHANICS TO UNDERSTAND AND MODEL SIMPLY AND EFFICIENTLY IN-SERVICE FAILURES

Wassim Taleb[*1] and Laurent Ponson*[1]

[1]*Tortoise*

ABSTRACT

Failure during service often results from a mismatch between the assumptions made by design engineers during the development phase and the realities of in-service conditions. Typically, either the applied load has been underestimated, or the actual material resistance has been overestimated. Despite the critical importance of this information, no current technique can measure material resistance and applied load simply and directly after an in-service mechanical failure.
We propose a disruptive method of failure analysis based on the statistical analysis of the fracture surfaces of components that have failed in service. This method, known as statistical fractography, extracts the material failure properties and the loads applied to the component at failure from the roughness features of the fracture surface. It provides a simple and rapid experimental methodology to measure the input data required to simulate an in service failure. In practice, the material failure properties and failure load measured from the scan of the fracture surface are used as inputs for fracture mechanics models, which then create numerical twins of the in-service failure.

This innovative approach is used to understand and describe failure scenarios in complex mechanical systems, offering a powerful tool to rationally redesign structures with enhanced failure resistance and longevity. Ultimately, this technique opens new perspectives for mastering the durability and reliability of mechanical components with unprecedented performance. In my talk, I will illustrate these methods through several examples of failure analysis.

Advanced materials: Computational analysis of properties and performance
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PENETRATION RESISTANCE OF GRAPHENE COATED CERAMIC MATERIALS UNDER PROJECTILE IMPACTS

Mohammad Reza Talebi Bidhendi[*1] and Kamran Behdinan*[1]

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ABSTRACT

Extreme conditions including impact can result in material degradation, permanent damages, and occasionally property/life loss. Therefore, investigation of materials and structures under projectile impact has been a canonical field of research over the past decades. Such studies have led to the development of hybrid materials with high performance and durability under the aforementioned loading. As an emerging hybrid material, graphene oxide (GO)-silicon carbide (SiC) provides promising thermo-chemo-mechanical properties with various applications in defense, energy, and aerospace engineering. Nevertheless, penetration resistance of such composites under impact received less attention due to experimental and computational difficulties. Here, ReaxFF molecular dynamics is leveraged to address the aforesaid problem. Accordingly, the response of 4H-SiC thin films coated by GO samples under indentation and high-velocity projectile impact is studied. It is observed that (a) ceramic substrates coated by GO samples with higher oxidation degree demonstrate softer behavior under indentation, and (b) fracture pattern and penetration resistance under high-velocity impact are dependent on the oxidation degree of the coating layers. In essence, impact-induced complete perforation is more localized to the impacted region as oxidation degree of the coating layers increases. Therefore, oxidation content can be deemed as a novel tuning factor for the fracture behavior of the GO-SiC thin films subjected to projectile impacts. The influence of oxygen functional groups on the adhesion energy between GO and SiC layers is also investigated. It is found that adhesion energy between SiC and the coating can be modified by the oxidation degree of the graphene samples. Eventually, the findings of this study reveal some insights into the bottom-up design pathways for developing novel ceramic-based protective barriers in which GO is used as a coating layer or reinforcement.

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Recent advances in indirect structural health monitoring
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ON THE CROWDSENSING-BASED OPERATIONAL MODAL ANALYSIS OF BRIDGE STRUCTURES USING PREDICTED RESPONSES WITH MISSING VALUES

Mohammad Talebi-Kalaleh[*1] and Qipei Mei*[1]

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ABSTRACT

The development of intelligent solutions for condition monitoring of infrastructures represents a pivotal stride toward realizing smart cities. Bridges, critical components of public transportation systems, are deteriorating due to various factors. This underscores the critical importance of vigilant monitoring and maintenance practices to ensure their structural stability and long-term performance.
Current indirect bridge monitoring techniques, relying on single or multiple passages of a sensing vehicle, have shown promising results as a low-cost alternative to traditional methods using fixed accelerometers. However, these methods face challenges in eliminating road roughness effects and continuously monitoring bridges due to limited interaction time between the sensing vehicle and the bridge, resulting in insufficient vibration data collection.
This research introduces an innovative crowdsensing-based method to identify the mode shapes and natural frequencies of bridges by applying the frequency domain decomposition technique on the vibrational data with missing values, considering road roughness and measurement noise effects. The proposed method employs a random selection approach among a network of sensing vehicles. Leveraging vertical and rotational acceleration data, along with GPS location data, enables predicting the bridge's sparse responses at virtual fixed sensing nodes. A primary innovation lies in using randomly selected sensing vehicles at each timestamp, overcoming data length limitations with a multi-agent approach for real-time data collection. Moreover, the method is robust to road roughness and operational effects, known to impact indirect bridge health monitoring techniques, by utilizing residual responses from the selected agents' rear and front axles.
Comprehensive numerical studies evaluated the method's performance, simulating a 2D bridge subjected to random traffic flow with two-axle vehicles. Numerical analyses, considering vehicle-bridge interaction, demonstrate the proposed method's efficacy in accurately identifying the first three mode shapes and natural frequencies of bridges. Notably, the method achieves over 95% accuracy in identifying the bridge's first three mode shapes and less than 5% error in identifying its natural frequencies.

Modeling and simulation of advanced manufacturing processes for metals
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODEL FORM SELECTION IN THE INDENTATION PLASTOMETRY INVERSE PROBLEM

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ABSTRACT

Can the performance reliability of additively manufactured metal components be predicted? Fatigue and fracture are highly sensitive to sample microstructure and the distribution of plastic deformation. Typical microstructure-sensitive models of metal deformation require microstructure generating statistics and instantiation of an ensemble of statistically representative volume elements. The common approach is difficult to apply to additive manufacturing processes due to two additional complications: (1) microstructure can vary spatially in a component due to process variations, and (2) property variations and geometric features are often on the same length-scale and are not separable as in the traditional problem formulation. What data can be used to select a model of heterogeneous plasticity between the single crystal and the homogenized length scales?

To capture the complexity of these new microstructures, local data sources will be crucial. Indentation plastometry can provide a local, physical homogenization of material properties with a flexible length scale of observation. Due to the challenge of interpreting material properties from the non-homogeneous loading conditions in indentation tests, material heterogeneity is often neglected in micro-indentation. However, nano-indentation of single crystals has been used to calibrate parameters of crystal plasticity constitutive models [1]. In all cases that use finite element simulations to aid the interpretation of experimental observations (of indentation profilometry and/or load-displacement curve), an inverse simulation problem is used. I.e., the unknown parameters of the material model are evaluated by minimizing error between the simulated data and the experimental data.

In this work, the process of selecting a plasticity model form from alternatives is determined. Data from 84 profilometry-based indentation plastometry tests of Al 7075 plate are used. Three macroscale plasticity model forms are used to replicate the data via finite element simulations. Bayesian ensemble approach [2] is used to determine parametric uncertainty in different model forms. A model selection procedure is developed that operates in model output space, such that the model selection can be performed in like-terms. A surrogate model is employed to accelerate the analysis. This new model selection will enable the development of new plasticity models for advanced processing applications.

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Towards predictive digital twins: Innovative algorithms for physics-, data-assisted and hybrid modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-INFORMED UNCERTAINTY QUANTIFICATION FOR LASER-BASED POWDER BED FUSION ADDITIVE MANUFACTURING BY MULTI-FIDELITY SURROGATE MODELING

Mihaela Chiappetta[1], Chiara Piazzola[2], Lorenzo Tamellini[3], Alessandro Reali[1], Ferdinando Auricchio[1] and Massimo Carraturo[1]*

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[2]*Technical University of Munich*
[3]*CNR-IMATI*

ABSTRACT

We present an efficient approach to quantify the uncertainties associated with the numerical simulations of the laser-based powder bed fusion of metal processes. Our study focuses on a thermomechanical model of an Inconel 625 cantilever beam, based on the AMBench2018-01 benchmark proposed by the National Institute of Standards and Technology (NIST). The proposed approach consists of a forward uncertainty quantification (UQ) analysis of the residual strain of the cantilever beam given the uncertainty on some of the parameters of the numerical simulation, namely the powder convection coefficient and the activation temperature. The uncertainty on such parameters is modeled by a data-informed probability density function (PDF) obtained by a Bayesian inversion procedure, based on the displacement experimental data provided by NIST. To overcome the computational challenges of both the Bayesian inversion and the forward UQ analysis we employ a multi-fidelity surrogate modeling technique, specifically the multi-index stochastic collocation method. The proposed approach allows us to achieve a 33% reduction in the uncertainties on the prediction of residual strains compared with what we would get basing the forward UQ analysis on a-priori ranges for the uncertain parameters, and in particular the mode of the PDF of such quantities (i.e., its "most likely value"', roughly speaking) results to be in good agreement with the experimental data provided by NIST, even though only displacement data were used for the Bayesian inversion procedure.

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Methods for identification, machine learning, and uncertainty quantification of reduced order models of coupled systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NOVEL DAE-ROM FRAMEWORK INTEGRATING ARBITRARY SPATIAL AND TIME DISCRETIZATION METHODS IN MULTIPLE SUBDOMAINS WITHIN A SINGLE ANALYSIS

Kumar Tamma[1] and David Tae*[2]

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ABSTRACT

Over the years, the development of numerical simulation computational framework has grown. Various space discretization methods such as finite element method, meshless methods, and particle methods and so on have been built. Concurrently, many researchers have upon worked numerous space and time discretization methods. Zhou and Tamma developed Generalized Single Step Single Solve (GSSSS) family of time integration algorithm[1] to embrace well known time integration algorithms as well as more new and novel schemes with improved physics such as energy-momentum conservation and numerical dissipation control while maintaining second order accuracy in time. They, later, extended the algorithm to first of system with the development of isochronous time integrators [i-Integrators].

There also has been a high interest in coupling subdomains which allows local control of analysis for computation efficiency. Here, we provide a novel representation of particle methods named, generalized particle system (GPS) method, and the FEM in a generalized setting for space; and for the time, we also propose integration of a novel subdomain DAE-ROM framework and the well-known GSSSS time family of algorithms for dynamic systems[2]. A variety of spatial and time-discretized methods and algorithms can be employed within a single analysis. The versatility of the GSSSS family of algorithms and its improved physics proves extremely useful to the subdomain framework. Coupling of different spatial and different time integration methods will allow for the selection of an appropriate method exploiting its advantages for localized subdomain areas. The flexibility, robustness, and reduced order modeling of the presented DAE-ROM framework is not possible with existing technologies that show limitations such as reduced order accuracy, limitations of flexibility, robustness, versatility and the like, including preserving a consistent second-order time accuracy in all variables such as displacement, velocity, acceleration and Lagrange variables.

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Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A BOND-BASED PERIDYNAMICS MODELING OF POLYMERIC MATERIAL FRACTURE UNDER FINITE DEFORMATION

Caglar Tamur[*1] and Shaofan Li*[1]

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ABSTRACT

We have developed a bond-based peridynamics model to study the fracture of polymer networks under finite deformation. Our approach is based on the Kuhn-Grün model of randomly jointed polymers with extensible chains, which allows the rupture of polymers through the chain scission mechanism. We introduced a novel mesoscale potential function into a nonlocal continuum framework with the purpose of modeling the mechanical response and fracture of polymers. We have demonstrated through a series of numerical examples, both two-dimensional and three-dimensional, that the proposed model is robust and efficient in modeling crack growth in polymeric materials. The model is carefully validated with experimental data and numerical results obtained on the basis of existing continuum mechanics polymer models. We have shown that the proposed peridynamics model is accurate and stable in various configurations and loading modes, such as mode-I and shear crack opening. In comparison to existing continuum polymer models and fracture modeling methods, our technique has the advantages of being theoretically simple, rigorous, and computationally fast. The numerical results show that the nonlocal polymer model can easily capture the fracture process in polymeric materials without complex ad hoc modeling parameters under finite deformation, and it has the potential to become a convenient simulation tool for modeling the polymer failure process in the design and optimization of polymeric materials.

Uncertainty quantification and scientific machine learning for predictive modeling of complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICS-CONSTRAINED LEARNING FOR PDE SYSTEMS WITH UNCERTAINTY QUANTIFIED PORT-HAMILTONIAN MODELS

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ABSTRACT

Modeling the dynamics of partial differential equation (PDE) systems plays a pivotal role in making safe and efficient control decisions as it allows us to forecast the future state of the systems. The applicability of such models extends across various domains. In particular, soft robots have gained popularity due to their ability to navigate complex and dynamic environments with greater adaptability and safety compared to traditional rigid robots. Their flexible and deformable structures make them well-suited for tasks such as medical procedures, search and rescue missions, and collaborative interactions with humans. However, finding accurate PDE models of these robots is challenging because of the materials involved with highly nonlinear properties. Data-driven approaches seem promising for modeling soft robots as PDE systems but often neglect basic physical principles, which consequently makes them untrustworthy and limits generalization. In this scenario, predictive models learned only from the data might be able to provide reliable forecasts. Previously, physics-informed learning methods such as PINNs[1] have been introduced, but typically lack uncertainty quantification to indicate the reliability of the learned models. Recently, we introduced a physics-informed Bayesian learning framework[2] which, however, was limited to learning rigid body dynamics.

In this talk, we present a physics-constrained learning method that combines powerful learning tools and reliable physical models. Our method leverages the data collected from observations by sending them into a Gaussian process that is physically constrained by a distributed Port-Hamiltonian model. Based on the Bayesian nature of the Gaussian process, we not only learn the dynamics of the system, but also enable uncertainty quantification. Furthermore, the proposed approach preserves the compositional nature of Port-Hamiltonian systems which allows us to easily connect the model with models of the environment while maintaining physical correctness and uncertainty quantification.

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Advances in multi-scale, multi-material, and multi-component Topology Optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CONCURRENT MULTISCALE TOPOLOGY OPTIMIZATION USING COMMERCIAL CODES WITH DIRECT FE2

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ABSTRACT

Together with the rapid development in manufacturing technology, multiscale structural topology optimization presents opportunities for the design of components at both the structural and sub-structural scales. A few works on topological optimization based on FE2 computational homogenization to concurrently evolve the structure and sub-structure have been reported. However, significant expertise and coding are required in the conventional implementation of FE2. It is shown that multiscale FE2 optimization can be readily implemented on commercial finite element codes using the Direct FE2 approach. The multiscale analysis is carried out as a single topology optimization job on commercial FE software after 2 simple pre-processing steps with no coding required. Numerical example problems are solved using ABAQUS to demonstrate the proposed method for stiffness optimization. It is shown that Direct FE2 optimization takes only a fraction of the computational time required for optimization with a fine mesh and yet gives comparable optimized stiffness.

The phase field method for fracture: Theory, numerics, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELLING MOISTURE-ASSISTED FRACTURE AND LIQUID-SOLID IMPACT IN COMPOSITE MATERIALS USING PHASE FIELD METHOD

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ABSTRACT

Composite materials find increasing applications in aerospace and offshore wind energy sectors owing to their outstanding specific mechanical properties. Nonetheless, these materials face susceptibility to demanding conditions, including dynamic impact loading and environmental degradation. Notably, the high-velocity impact of liquid droplets can induce significant erosion damage to the leading edges of wind turbine blades. Phase Field (PF) fracture models emerge as promising solutions for anticipating such challenges. These PF methods adeptly capture diverse crack paths and evolving interfaces, seamlessly integrating with multiphysics phenomena. Moreover, the PF interface approach plays a crucial role in replicating the flow behaviour of two distinct, immiscible fluids, with a specific emphasis on accurately determining their interface position. This study aims to explore the influence of factors such as microstructure, moisture content, and dynamic liquid-solid impact on the material's macroscopic performance.

In this research, we introduce a numerical framework that integrates phase-field fracture modelling with moisture diffusion and hygroscopic expansion to forecast environment-induced failures in composite materials. Our model undergoes rigorous validation against experimental data, demonstrating proficiency in replicating moisture dispersion, fibre and matrix swelling, and fibre-matrix debonding. Expanding our computational framework, we proceed to simulate liquid-solid interactions, leveraging the Arbitrary Lagrangian-Eulerian (ALE) technique in conjunction with a predefined multiphysics interface for Two-Phase Flow and Phase Field. Comparative analyses of displacement, strain distribution, and historical strain waves affirm the model's accuracy in alignment with experimental findings. The computational architecture provides a virtual platform to explore microstructural features, material properties, environmental-induced degradation, and dynamic liquid-solid impacts. Such advancements are pivotal in optimizing designs, propelling the evolution of next-generation transport and offshore energy innovations

Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN AI ASSISTED WALL HEAT FLUX MODEL FOR FLAME-WALL INTERACTION IN TURBULENCE

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ABSTRACT

Flame-wall interaction (FWI) is a widely encountered phenomenon in combustion devices where the combustion occurs in an enclosed chamber. It is typically characterized by a pronounced decrease in flame reactivity (near-wall flame quenching) and a substantial level of quenching-induced wall heat flux which critically impacts the thermal efficiency of combustion devices. Currently, despite active research into FWI through Direct Numerical Simulations (DNSs) and experimental approaches, the highly localized and reaction-coupled nature of FWI presents ongoing challenges for its accurate modeling.

In response to these challenges, this study introduces a machine-learning-based Large Eddy Simulation (LES) model designed to predict wall heat flux resulting from FWI. The model is trained on a DNS dataset of premixed methane-air combustion in constant volume vessels across various flow conditions, including 1D laminar, 2D laminar, and 2D turbulent flows. It is trained with the neural network, considering the time-integrated value of the wall heat flux as the output quantity and the flame-wall distance, integration time, and other wall-heat-transfer-related thermochemical quantities (e.g. mean pressure and the ratio of preheat temperature to wall temperature) as the input quantities. Additionally, the model incorporates flame-wall geometric features by including the angle between the flame and the wall in the input layer. All input and output quantities are appropriately non-dimensionalised and scaled numerically based on the maximum of their absolute values. The Adam optimization method and mean squared error loss function are utilized in the model training process.

The current results from the DNSs of current combustion scenarios indicate a strong dependence of FWI-induced wall heat flux on the flame-wall distance, as well as on thermodynamic states including preheat temperature, wall temperature, equivalence ratio, and initial pressure. Correspondingly, the AI-trained model demonstrates robust predictive performance for wall heat flux during near-wall combustion under various flow conditions, as evidenced by a notable decrease in the loss function value during machine learning training and a correlation coefficient exceeding 0.9 when comparing model-predicted to original DNS wall heat flux values. The current study underscores the potential and promise of employing machine learning methodologies to develop advanced models for wall heat transfer in combustion systems.

Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SPECTRAL DECOMPOSITION BASED NATURAL STABILIZED NODAL INTEGRATION FOR HIGHLY ORTHOTROPIC AND NEARLY INCOMPRESSIBLE MATERIALS

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ABSTRACT

Nodal integration (NI) methods are of great interest in meshfree methods because they are simple and require less computation to integrate the weak form. However, a naive application of NI such as direct NI (DNI) usually results in an unstable and inaccurate formulation due to spurious singular modes. Recently, naturally stabilized nodal integration (NSNI) has been proposed by Hillman and Chen [1] to eliminate the unstable modes with a minimally additional cost compared to DNI. Overall, NSNI is a highly efficient and accurate integration scheme widely used in various problems. However, when we applied NSNI to applications related to highly orthotropic and nearly incompressible materials, we realized that the displacements were usually underestimated by large factors, especially for small nodal support sizes. Hence, an improved NSNI is introduced to overcome the locking issues encountered by the standard counterpart. The elasticity matrix is known to have stiff modes associated with high eigenvalues for highly orthotropic and nearly incompressible materials. Since the standard NSNI contains the full elasticity matrix, it may provide improper stabilized energy, which causes locking. Therefore, the proposed method utilizes spectral decomposition [2] to identify stiff modes in the elasticity matrix. Then, terms associated with stiff modes in the weak form are integrated by NI without stabilization, whereas NSNI is introduced for the other terms. Several two- and three-dimensional numerical examples are tested to demonstrate that the proposed approach enhances the capability of NSNI to deal with displacement locking.

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Novel numerical approaches for integrated disaster simulation for digital twin from living spaces to urban scales
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SEQUENTIAL UPDATING OF BUILDING FRAGILITY FUNCTIONS THROUGH LARGE-SCALE SEISMIC SIMULATIONS AND SENSOR INTEGRATION

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ABSTRACT

This study introduces a framework for assessing the seismic risk of urban buildings, specifically in Sendai City, Japan. It integrates city-scale numerical simulations with sensor data to evaluate earthquake responses of buildings. The methodology focuses on developing and refining building-specific fragility functions using numerical simulations, enhanced by sensor data integration. The Proper Orthogonal Decomposition (POD) technique plays a crucial role in optimizing sensor placement for maximum efficiency and minimal quantity, to circumvent practical constraints in urban environments.

A critical part of the research is applying POD to analyze numerical simulation data. POD is a method that identifies principal components from numerical simulation data, enabling effective data decomposition and reconstruction. This approach helps represent large-scale simulation results in a more compact and meaningful way, a crucial step in comprehending seismic impacts. Besides, the framework also highlights the importance of sparse sensor distribution [1]. The study strategically places sensors to maximize data collection efficiency while minimizing the number of sensors. This optimization is vital for practical use in urban areas, where large sensor networks may be impractical.

Also, the study uses cloud analysis [2] and Bayesian updating [3] in a novel manner. It first creates fragility functions for all buildings together based on cloud analysis using numerical simulation data, Cloud analysis uses the linear regression in the logarithmic scale by least squares to establish the relationship between engineering demand parameter (EDP) and intensity measure (IM), and then progressively refines them by incorporating sensor data through Bayesian inference. This dual-stage approach allows for a rapid safety assessment of all buildings in a given area, with continuous improvements to the fragility functions by the accumulating sensor data.

This research offers valuable insights into seismic impacts and mitigation strategies, particularly relevant for earthquake-prone area such as Sendai city. It contributes to urban seismic risk management, providing methodologies that strengthen earthquake preparedness and resilience in urban areas worldwide.

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Uncertainty quantification and scientific machine learning for predictive modeling of complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODEL SELECTION AND DIMENSION REDUCTION OF CHEMICAL KINETICS MODELS FOR TURBULENT COMBUSTION

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ABSTRACT

Our ultimate goal is to simulate the interaction between supersonic turbulent combustion and composite materials in complex geometries. Validation of such simulation models is particularly challenging in part due to the many sources of uncertainty present in the integrated model. This work focuses on combustion kinetics models, whose uncertainty has a significant impact due to the nonlinearity of Arrhenius models.

A set of candidate kinetics models is shortlisted based on their efficiency and anticipated accuracy. A probability distribution is assigned to Arrhenius parameters, which represents the primary source of uncertainty in a kinetics model. We then develop a model selection approach to select the best available mechanism for our particular combustion applications. There is a challenging balance between model complexity and model prediction power. More calibrated parameters will typically allow a model to better reproduce data. However, a model that is 'overfitted' will not extrapolate well. Formal model selection statistical analysis provides a route to balancing these two factors to suggest a model that is justified based on the available data for calibration but still not slavishly linked to it so much that the underlying physics of the model become secondary to the goodness of fit. We demonstrate our model selection approach and select the most plausible mechanism using the standard combustion software tool Cantera for a case of axisymmetric flames stabilized at a stagnation point.

Once the most plausible kinetics model is selected, a remaining significant challenge is the curse of dimensionality when uncertainty quantification and validation are performed for large-scale turbulent combustion simulations. Global sensitivity analysis is a standard approach to focus on the most influential reactions. One drawback is that an arbitrary threshold is often required. When reactions are comparable between each other, threshold-based selection is not always viable. We propose a novel method for dimension reduction, which considers the number of uncertain parameters as model classes, as in a model selection approach. This method takes advantage of experimental data for selecting the most important reactions and avoids a user-given threshold. We will use an axisymmetric configuration of ethylene-hydrogen-air flat flame on a McKenna burner to assess our dimension reduction approach. The simulation is performed using the in-house developed multiphysics software framework MIRGE-Com.

Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MICRO-MESO COUPLED MODEL FOR CORAL REEF ROCKS BASED ON CT SCANNING

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ABSTRACT

The coral reef rock has a rich porous structure, and establishing a entity model with a realistic porous structure will do great good to study the mechanical behavior and its mechanisms. However, the pore's characterized size of coral rocks span four orders of magnitude from micro to meso scales (1μm to 10mm). Large pores require the size of a specimen to be sufficiently large, while small pores request the element size in the model to be very small. The selfconflict sizes of specimen and element result in an enormous number of elements in the entity model to lead to extremely high computational costs. To overcome this fundamental challenge, this paper uses CT to scan a macro coral specimen to obtain an entity model and establishes a dual scale coupled model: (1) retaining pore's equivalent diameter larger than 1mm in the overall CT entity, and regarding the rest part as a uniformly dense matrix material with unknown material's properties, which is called the meso model; (2) extracting a small entity containing pore's equivalent diameter less than 1mm from the CT entity, which is called the micro-scale model also with unknown matrix material properties; (3) the unknown matrix material parameters in meso model are derived from mechanical response of the micro model, and the unknown matrix material parameters in micro model are confined by that meso model's mechanical responses should be coincident with that of a resl coral specimen. This micro-meso dual scale coupled model retains the influence of pores at various scales, and a computational result shows that it can reduce the computational complexity of a single CT entity model by four orders of magnitude. It provides a new approach for studying similar materials' mechanical behavior and mechanisms under complex loading conditions.

Computational mechanics in Canada and China: Current states of shared scientific interests and opportunities for the future cooperation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA DRIVEN POLYMER CONSTITUTIVE MODEL BASED ON PRIOR KNOWLEDGE OF MECHANICS

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ABSTRACT

Traditional constitutive models for polymers have achieved remarkable results over the years, with the advantages of fewer control parameters and clearer physical meanings of the parameters. However, the building of these models is complex and time-consuming, relies on a large amount of experience, and is difficult to keep pace with the development of new materials. Data-driven constitutive modeling methods based on data processing and analysis have developed rapidly. However, existing research in this field usually treats methods such as machine learning as a black box for data processing, ignoring the prior knowledge of mechanics accumulated over a long period of research. Thus requires the support of a huge amount of data in order to obtain an accurate material constitutive model. This report presents our recent research work that enables viscoelastic/viscoplastic constitutive modeling and computational methods for polymers using less data requirements driven by combining solid mechanics mechanisms with data-driven computational methods. Our method has several advantages: (1) it eliminates the interference of human experience by automating the establishment of constitutive relationships through data, which greatly improves the efficiency of establishing new material constitutive; (2) it effectively combines mechanistic mechanisms, and the amount of data required is much smaller than that of a purely data-driven method, which improves the practicability of the method; (3) it can be conveniently integrated into Abaqus, which is easy to use. These advantages give our method a wide range of applications in the field of material constitutive modeling.

Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ONLINE UPDATE OF DIGITAL TWIN AND ITS APPLICATION TO METAL ADDITIVE MANUFACTURING

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ABSTRACT

Digital twin (DT) refers to any model with capabilities to predict responses of physical systems and update online based on measured sensor data from physical systems. Depending on the type of DT models, online update methods could be classified into several categories. 1) The data-driven artificial intelligence models could be updated by changing model architectures and hyperparameters, whose relevant topics include lifelong learning, meta learning, and incremental learning. However, those methods suffer from the catastrophic forgetting problem, where the updated model would lose information about previous data. 2) The unknown system parameters of partial differential equations (PDEs) (i.e., dynamic systems) could be updated online by optimization, inverse engineering, statistics, or Kalman filters. Although those methods have been studied widely in hybrid simulations and data assimilation tasks, they are designed based on PDE functions which are not always accessible in all engineering tasks. 3) The proper orthogonal decomposition based reduced order models (POD-ROM) can adjust the number of reduced modes and update corresponding mode coefficients by incremental computation, which keeps prediction accuracies of previous data and new sensor data simultaneously. However, the accuracy of previous data is less important during applications, as the online sensor data may differ from the previous data even on the same input conditions.

Given the fact that PDEs of physical systems are not always available, and the update is based on an existing DT which is supposedly representing the current physical system, it seems the third category of update approaches is most promising for online DT updating. This work thus focuses on developing DT update methods based on POD-ROM. By fixing the first n modes and mode coefficients, the update of remaining modes and relevant coefficients are defined as a pseudo dynamic system which is extracted from the POD process and incremental computation process. Kalman filter series are then applied to update the remaining modes and coefficients to increase the online prediction accuracy with increasing online sensor data.

The proposed method is tested in metal additive manufacturing, where the temperature field of the yet-to-print layer is reconstructed by POD-ROM. As simplifications (e.g., no geometry deviation) are applied during modeling, POD-ROM would fail to provide accurate feedback to support the process control for the current layer. Based on the proposed online update method, the offline POD-ROM is tuned with the sensor data of same points during printing, improving the prediction accuracy for the layer at future timesteps.

Advance and application of meshfree methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A VC/NON-VC COUPLED MATERIAL POINT METHOD FOR STRUCTURAL FRAGMENTATION PROBLEMS WITH PHASE FIELD METHOD

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ABSTRACT

Meshfree methods, such as the material point method (MPM), can effectively handle material fragmentation problems, bypassing mesh distortion and separation that is deleterious to the conventional mesh-based formulation like finite element method. In addition, by incorporating proper fracture mechanics into Galerkin formulation, such as phase field method, one can easily track the fracture domain under variational principle. The well-known cell-crossing instability and loss of Galerkin exactness can be mitigated by our recently developed VC-RK material point enhancement [1], where the cell-crossing is overcome by using a smooth reproducing kernel (RK) approximation and the loss of Galerkin exactness is remedied by introducing the variationally consistent (VC) correction. However, during material fragmentation, dealing with the boundary integral within the VC framework becomes challenging due to the presence of newly generated surfaces. To achieve a robust simulation in fragmentation problems, the deformation-based coupling scheme [2] is introduced in the Galerkin MPM to couple VC (for continuum bodies) and non-VC (for discrete bodies), and proper stabilization is introduced to ensure the stability in the non-VC portion of the problem. The stabilized MPM framework is proven effective through benchmark examples with extreme deformations, assessing its consistency and stability.

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Physical models and reduced order models augmentation with data for physics-informed machine learning in real-world applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFICIENT DIGITAL TWIN OF COMPLEX MATERIAL BEHAVIOR THROUGH MACHINE LEARNING-ENHANCED NONLINEAR HOMOGENIZATION

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ABSTRACT

Nonlinear homogenization, as explored in [1], has proven to be a dependable approach for deriving macroscopic constitutive relations and field statistics in two-phase composite materials. The method is based on an optimal linearization of the nonlinear composite, leading to the best linear comparison composite with identical field statitics than the nonlinear material and which properties can be estimated with standard linear homogenization methods. However, as the fidelity of the physical representation of the material improves, the associated calculation time increases, thereby limiting the practical implementation of nonlinear homogenization methods in commercial finite element software for larger scale structure calculation.

To address this challenge while maintaining both precision and efficiency, machine learning can be leveraged to construct a digital twin of the composite constitutive law. This approach allows predicting macroscopic material behavior in real time, while ensuring accurate results.
The robustness of this method has been demonstrated for two-phase composites with nonlinear power-law constitutive relation, and it has been successfully extended to model the more intricate three-dimensional behavior of viscoplastic polycrystals. In the latter case, there is a substantial reduction in computational time without compromising the precision of nonlinear homogenization methods.

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Transport phenomena in micro/nanofluids
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ELECTRIC-FIELD-INDUCED ION EVAPORATION FROM THE IONIC LIQUID-VACUUM INTERFACE

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ABSTRACT

We studied ion evaporation from a planar interface between the room-temperature ionic liquid (RTIL) and vacuum under external electric fields by using molecular dynamics (MD) simulations. We calculated the ion evaporation rate (je) as a function of the electric field normal to the RTIL surface (En), and results under Langevin, dissipative particle dynamics (DPD), and Berendsen thermostats were compared. It was found that DPD thermostat is more suitable for simulating the ion evaporation phenomenon. We also compared results under different methods for applying the electric field (constant potential, constant charge, and constant field methods) and found that je-En curves from the three methods agree with each other. Temporal evolution of electric fields in vacuum was further analyzed, and variations of electric fields over time were traced to the induced electric field between the evaporated ion and RTIL film. This work could guide the selection of proper methods for MD simulations of electrospray in the pure ion regime and lays the foundation to study more complex electrospray phenomena using MD simulations.

Advances in material model calibration for computational solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A CALIBRATION STRATEGY FOR PROGRESSIVE INTEGRATION OF NEW CREEP EXPERIMENTS FOR SALT ROCKS

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ABSTRACT

The storage of green hydrogen in salt caverns requires fast injection and production rates to cope with the imbalance between energy production and consumption. This raises concerns about the mechanical stability of salt caverns under such operational conditions, which requires careful planning, often using numerical simulations. However, the accuracy of simulations is strongly dependent on the choice of a suitable and appropriately calibrated constitutive model. Salt rocks present a complex mechanical behavior, with different time-dependent deformation mechanisms simultaneously taking place [1]. As a result, constitutive models for salt rocks tend to depend on many material parameters, for which automated calibration strategies are often employed. Moreover, as pointed out in [2], inherent differences between samples of the same batch and difficulties in experimental controls constitute additional challenges to the calibration process, as a large set of experimental results should be employed to obtain a single set of representative material parameters. However, creep experiments are usually time-consuming, implying that the size of experimental datasets increases at a low pace. Therefore, it would be convenient to perform partial calibrations with the experimental data currently available and incorporate new experiments as they become available. During this process, the quality of the model results should increase as more experiments are used for calibration, and it should stabilize when a sufficient number of experiments is reached.

In this context, we present a progressive calibration procedure that incorporates one experiment at a time by properly adjusting an objective function and solving it as a multi-objective function optimization problem. Moreover, a regularization term is added to the loss function to roughly favor the same fitting quality for all experiments. The Particle Swarm Optimization (PSO) algorithm is employed to solve the optimization problems. Additionally, we investigate a situation where each experiment is performed on salt samples with slightly different material properties, for which the goal is to find a single set of representative material parameters. The results show that the proposed calibration strategy is robust and provides increasingly better predictions as more experiments are available for calibration.

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Physics-based data-driven modeling and uncertainty quantification in computational materials science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEEP LEARNING FOR MODEL CORRECTION

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ABSTRACT

Despite many recent advances and new deep learning technologies, training of the Deep Neural Networks (DNNs) for modeling of unknown systems generally requires large amounts of high-fidelity training data. Such large quantities of data may not be available in many practical applications, hence it is of importance to develop methodologies that can accurately correct imperfect prior models given scarce amounts of high-fidelity data. Hence, utilizing the Flow-Map DNN methodology and transfer learning, we present a model correcting framework and demonstrate its effectiveness on several numerical examples.

Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL STUDY ON MODELING OF ICE CRYSTAL ICING WITH CONSIDERATION OF ICE EROSION PHENOMENON.

Wakana Tatsuta[1], Koji Fukudome*[2], Soichiro Fujimura[1] and Makoto Yamamoto[1]*

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ABSTRACT

Many experiments and numerical simulations have been conducted to predict ice accretion, as its occurrence on an aircraft poses a threat to the safety and stability of the aircraft during operation. Ice crystal icing is a phenomenon of ice accretion that occurs in aircraft engines. It leads to engine power loss due to the ice layer formation by impinging ice particles on the fan and compressor walls. However, as the mechanism behind ice crystal icing is not yet fully understood, modeling of ice crystal icing remains an urgent issue. Recent experiments on ice crystal icing have unveiled phenomena such as sticking, bouncing, and erosion by the conditions of the impinging ice particles. Understanding the behavior of ice particles during impingement is crucial for accurately predicting the ice shape in ice crystal icing. While ice crystal icing models incorporating the effects of sticking and bouncing have been developed in recent years, only a limited number of models account for ice erosion.

This study introduces a novel ice crystal icing model by incorporating an ice erosion model. The icing simulation comprises four steps: flow field computation, ice particle trajectory computation, thermodynamic computation, and grid modification. The proposed ice erosion model is integrated into the thermodynamic model based on the extended Messinger model [1]. The erosion model for the accreated ice was derived from a semi-empirical model employed in predicting sand erosion based on classic solid/solid collision theory [2][3]. The parameters for this semi-empirical model were selected based on the impacts of ice particles on the ice layer and the melting ratio of the impacting ice particles. Numerical simulations of ice crystal icing were conducted under various conditions using the ice erosion model. The results revealed a significant discrepancy in the predicted icing shape depending on the presence or absence of the erosion model. In addition, the model was also validated through comparison with experimental data.

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Mesh-free particle methods for multi-physics problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A FLUID-STRUCTURE INTERACTION MODEL USING MOVING PARTICLE SEMI-IMPLICIT (MPS) METHOD

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ABSTRACT

Fluid-structure interactions (FSI) play a crucial role in civil engineering, shaping the resilience and optimal design of structures facing intricate forces. This paper presents an accurate and efficient fully-Lagrangian FSI model based on the Moving Particle Semi-Implicit (MPS) method. The simulation algorithm solves the governing equations of fluid and solid mechanics using separate two-way coupled MPS models. The coupling scheme is streamlined by adopting the mesh-free method (MPS), eliminating challenges associated with meshes while maintaining accuracy comparable to conventional mesh-based models. The solid model accounts for nonlinear structural dynamics and a failure mechanism in solid materials. Computational efficiency is achieved through parallelization as well as an innovative neighbor search strategy. Modified particle-shifting and interface detection methods enhance the simulator's capability to capture complex interactions.

To validate and evaluate the model's performance, we conduct comprehensive benchmark comparisons for various conditions, including solid-only models (e.g., free vibration of a cantilever thin plate), fluid-only models (e.g., dam break flow), and different FSI scenarios such as dam break flow against an elastic wall. Stability, computational efficiency, and accuracy of the results are evaluated against the available analytical and experimental data, proving the capability of the developed model.

A HYBRID LATTICE BOLTZMANN APPROACH FOR PARTICLE-LADEN FLOWS WITH THE PRESENCE OF FOULING LAYERS

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ABSTRACT

We this study, we focus on exploring hybrid lattice Boltzmann methods for simulating particle-laden flows, particularly to model calcium carbonate scale formation in high Reynolds number environments. Accurately modeling these particle-laden flows with fouling layers is challenging due to the need to balance model complexity and computational feasibility. Factors such as particle size, shape, density, and chemical composition significantly influence flow dynamics and fouling layer formation. Developing comprehensive models that encompass all relevant physical effects is impractical, necessitating the proposal of more manageable yet effective models. Correlating these models with experimental data presents its own set of challenges, highlighting the need for precise calibration tools. Such tools require a significant number of simulations to ensure accuracy in the results. To balance computational efficiency and accuracy, we propose an improved combination of phase-field models with Eulerian-Eulerian descriptions of particle motions. Additionally, for the proposed set of equations, we introduce a numerical solution based on a hybrid formulation of the lattice-Boltzmann method. We also discuss comparisons with Eulerian-Lagrangian schemes, and when possible, we compare the results with experimental data, using data assimilation enhanced by Bayesian inference tools.

Modern structure-preserving methods for PDEs
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ENERGY AND ENTROPY STABLE HIGH-ORDER CUT DISCONTINUOUS GALERKIN METHODS

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ABSTRACT

We present results on energy and entropy stable frameworks for high-order discontinuous Galerkin methods on cut meshes. Cut meshes provide the ability to represent complex geometries while maintaining the simplicity of a Cartesian mesh wherever possible. However, cut elements present two issues due to their arbitrary size and shape: the possibility of a severely restricted CFL condition and difficulty in generating exact quadrature. In the energy stable case, we show that state redistribution can be used to address the small cell problem while maintaining L2 stability. For entropy stability, which requires exactness guarantees on quadrature, we use curvilinear triangulations and Caratheodory pruning to generate sufficiently exact but still computationally efficient quadrature on cut elements. We present initial results applying these frameworks to the acoustic wave and compressible Euler equations, respectively.

Physics-based data-driven modeling and uncertainty quantification in computational materials science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOWARD ESTABLISHING A REDUCED ORDER AND SURROGATE MODEL FOR RESIDUAL STRESS IN ADDITIVE MANUFACTURING

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ABSTRACT

The high thermal gradients and fast thermal cycles associated with additive manufacturing (AM) lead to residual stress development during solidification, which has a deleterious effect on the long-term structural integrity of AM components. Further, the small length scale of AM components, such as the lattice struts or thin wall features commonly constructed, combined with the epitaxial growth of solidification causing large grain sizes, results in a coupling of length scales between the engineering length scale of the component and the scale of microstructural heterogeneity. This motivates the development of process-structure-property descriptive models resolved at the polycrystalline level to understand the effect of build condition parameters on microstructure features, and in turn, on material properties. Recently, a solidification model for laser powder bed fusion processing based on the cellular automata finite element (CAFE) was developed and validated against experimental electron backscatter diffraction data, and is capable of generating representative volume elements of solidified microstructures. When coupling this model with the crystal plasticity finite element model, the thermomechanical equations associated with laser processing can be solved to predict the mechanical response, which includes the effect of polycrystalline heterogeneity, at the microstructural length scales. While this modeling framework is capable of computing detailed, high fidelity mechanical response fields, it is prohibitively computationally expensive for parametric analysis or for simulations covering very large domains. Therefore, this work studies the applicability of hyper reduced order models (HROM), such as the energy conserving sampling and weighting algorithm, for identifying and constructing the low dimensional manifold over which the solution field resides. A distinct feature of AM solidification for HROM applications is the translating heat source, leading to the potential existence of a steady state solution. It is sought to exploit this feature by developing evolutionary reduced bases functions that are defined with respect to the translating laser source. One factor limiting widespread use of HROMs is that they are inherently intrusive, meaning that solving the online problem requires completely recoding the numerical implementation of the solution to the system of equations. In contrast, neural operator surrogate models are nonintrusive, yet they suffer from the large demand placed on optimization algorithms by searching over a large parameter space. This work studies integrating HROMs with neural operator networks such that neural network optimization is confined to the low dimensional manifold identified by the HROM. The new model will be formulated and its performance tested on example problems.

Imaging-based methods in computational medicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN AUTOMATED WORKFLOW FOR CONSTRUCTION OF VIRTUAL TWINS FOR HAEMODYNAMIC ANALYSIS OF STENOSED NATIVE AORTIC VALVES

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ABSTRACT

An ageing population and changes in demographics have brought valvular heart disease to a central focus in cardiovascular medicine. Aortic stenosis, accounting for 42% of valvular heart disease cases, is characterised by calcium deposits that narrow and stiffen the aortic valve, resulting in elevated transvalvular pressure, reduced blood flow, and increased cardiac workload. It is widely recognised that fluid-structure interaction (FSI) simulations offer the most accurate representation of the interaction between the aortic valve and its surrounding flow field, as well as associated pathologies [1]. FSI simulations, however, particularly involving complex, patient-specific geometries, present challenges such as time-consuming image-based anatomy reconstruction, complex meshing, long set-up times, and the difficulty of automation. We present an automated workflow designed to create virtual twins of the aortic root and conduct FSI simulations to analyse blood flow in stenosed aortic valves. While the focus here is on the simulation of native diseased valves, the workflow is designed with subsequent simulation of clinical interventions, such as transcatheter aortic valve implantation (TAVI), in mind.

Using computed tomography angiography (CTA) scans, echocardiography, and Doppler imaging data, patient-specific simulations of the valve haemodynamics are obtained using the workflow detailed below. Detailed models of the aortic root, including the aorta, left ventricle outflow tract, and calcifications, are generated from CTA scans. Valve leaflets, not directly obtained in segmentation due to limitations on imaging spatial and temporal resolutions, are inferred for each patient from detected anatomical landmarks. These steps are performed using SimplewareTM Software (Synopsys Inc, USA), and an in-house code. Fully coupled FSI simulations of the valve haemodynamics are then conducted for each patient. Using Ansys LS-DYNA, augmented with custom Python scripts, this process is applied to several patients to provide performance predictions for comparison with clinical measurements. The simulations provide information on pressure gradients across the valve; stress field and blood velocity, at peak systole and diastole; and calculations for blood flow rate, regurgitant volume, orifice area, and jet time-velocities. Model outputs are validated against Doppler traces.

This automated workflow, incorporating FSI simulations, aims to provide a tool for understanding the physiology of aortic stenosis and the underlying disease mechanisms. With further refinement, it can form a key building block of in-silico trials of cardiac devices and interventions.

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Computational modeling of cardiac fibrosis: A multiscale, multiphysics challenge
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MECHANICAL MODELING OF CARDIAC FIBROSIS WITH EXPLICIT SPATIAL REPRESENTATION OF MYOCYTE LOSS AND COLLAGEN ALIGNMENT

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ABSTRACT

Cardiac fibrosis is a pathological condition that decreases myocardial contractility and increases stiffness, leading to reduced cardiac function. One form, replacement fibrosis, occurs as damaged myocytes are replaced with stiffer collagenous tissue containing more aligned collagen fibers [1]. It remains unclear how different sub-processes individually contribute to the loss of cardiac function. In this work, we explored the mechanical microscale impact of various factors through a computational framework.

We employed a mechanical model allowing for explicit geometrical representation of individual myocytes embedded in extracellular matrix (ECM), also incorporating spatial representation of the collagen fibers. We assumed all cells to be aligned within the tissue block, while allowing for spatial variation of collagen. An active stress model was used to model cellular contraction.

Previous work [2] indicates that contractility and stress are locally dependent on the directionality of fibrosis progression. Expanding on these findings, we examined myocyte loss of 50% (64 out of 128 cells) progressing longitudinally, transversely, or randomly. We next used our framework to simulate the impact of myocyte loss in combination with other parameter changes, impacting myocyte/matrix stiffness and collagen alignment.

In our simulations, the impact of myocyte loss had the largest effect on resulting strain and stress – with up to 45% loss in strain and up to x7 higher stresses in the extracellular subdomain. Increased myocyte and matrix stiffness further reduced the strain (up to 12%). Meanwhile, collagen alignment in the myofiber direction increased strain, partially restoring the effect of myocyte loss (~5% restoration). Collagen alignment in the myofiber direction also reduced the extracellular stresses caused by myocyte loss (up to 45% and 25% restoration, respectively).

Our modeling framework effectively captures differences in stress and strain resulting from changes in spatial cellular configuration and extracellular collagen alignment. Myocyte loss in all scenarios led to reduced contractility and increased matrix stresses. Meanwhile, increased myofiber direction collagen alignment partially restored contractility and decreased matrix stresses, which may signal this is a compensatory mechanism to the loss of myocytes. Future endeavors integrating modeling frameworks with experimental data could build on this to gain deeper insight into factors of cardiac fibrosis.

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Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ACTIVE LUBRICATION INTERFACES WITH TUNABLE MICRO-TEXTURES

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ABSTRACT

Designing interfaces with the optimal operating conditions for hydrodynamic lubrication has been a vibrant research topic in the context of tribology. Since early studies, there has been an effort to design surface textures towards optimal load carrying capacity or friction behavior. Homogenization is a well-established methodology to account for the oscillatory response due to the micro-texture features of a design. This approach is based on the Reynolds equation that is commonly adopted to capture the physics of the thin film lubrication problems. Given such an approach, most design studies in the field are based on parametric frameworks which limit their ability to capture complex topological features. In this context, topology optimization is a widely invoked approach that may be suitably combined with homogenization to deliver an unrestricted design space. Moreover, the surface design does not need to be fixed in time. Manufacturing of smart surfaces have recently displayed significant development. The materials that such surfaces are composed of are not only tailored spatially but also display temporal changes according to an external excitation, such as for electric field-responsive surfaces. Such smart surfaces offer a potential for further optimizing the lubrication behavior, which is the focus of this work. Specifically, a space-time homogenization-based topology optimization approach will be invoked in order to design active surfaces which target objectives based on flux and traction. A novel unit cell optimization approach is additionally employed in order to remove configurational constraints from the optimization framework. The results obtained from this framework are then heuristically projected to generate 3D realizations of representative surface elements which respond to electric fields, thus morphing their surface textures. The macroscopic response of these preliminary realizations are subsequently compared against the original design predictions. Overall, this study is a first step towards a comprehensive design framework for active interfaces.

Computational fluid dynamics (CFD) and fluid-structure interaction (CFSI): Methods and Applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A POSITION-BASED FORMULATION OF THE PARTICLE FINITE ELEMENT METHOD FOR MONOLITIC SOLUTION OF FLUID-STRUCTURE INTERACTION CONSIDERING NEWTONIAN AND NON-NEWTONIAN FLOWS

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ABSTRACT

This work presents the application of a position-based formulation of the Particle Finite Element Method (PFEM) [1] applied to the monolithic solution of fluid-structure interaction problems considering free-surface incompressible Newtonian flows and non-Newtonian Bingham flows. The same motion description is adopted for both, fluid and solid domains, taking as main variable the current position, making the monolithic solution of the coupled problem straight-forward. However, as solids develop only finite strains, its description always takes the initial configuration as reference (total Lagrangian Description), while for the fluid, we allow the reference to be arbitrarily updated to any other configuration of equilibrium of the fluid domain, enabling partially or fully updated Lagrangian descriptions. For the solid, we consider the Saint-Venant-Kirchhoff elastic constitutive model. The principle of stationary energy is employed to get the weak solution for both, fluid and solid domains, so that it is written regarding current nodal positions for the solid and regard current nodal positions and nodal pressures for the incompressible fluid flow. The Newtonian constitutive model, as well as the Papanastasiou regularization that we adopt for the Bingham model, keep stresses independent of the deformation history. This makes updating the reference for the fluid simple, without the need for considering the stress distribution in the past reference. To deal with the undefined distortions that can occur in the fluid domain, as well as to allow topological changes, we adopt for the fluid domain the PFEM technique, that has as main characteristic considering a cloud of particles as nodes of a finite element discretization that is constantly reconstructed, justifying the updated Lagrangian description of the fluid. To circumvent the Ladyzhenskaya-Babuska-Brezzi restrictions, and allow linear interpolation for both, pressure and position, a pressure stabilizing Petrov-Galerkin technique is employed. The implicit α-generalized strategy is chosen to perform the time integration, enabling second order convergence and ensuring good stability due to the numerical dissipation control. A variety of selected 2D and 3D problems, including dam-break problems over elastic structures, flux valves, and concrete casting, are simulated to assess the formulation. The simulations demonstrate the robustness, versatility, and potential applications of the proposed formulation.

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Computational methods in environmental fluid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL ANALYSIS OF HOT AIR RECIRCULATION PHENOMENON USING MICRO-WEATHER MODEL, A COMPRESSIBLE LARGE EDDY SIMULATION

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ABSTRACT

Liquified natural gas (LNG) has been growing its demand as a low CO2 emission energy resource. Its production efficiency is strongly affected by the efficiency of heat exchangers in LNG plants. The Hot Air Recirculation (HAR) phenomenon, which occurs under specific weather conditions such as crosswinds, is one of the important factors that deteriorate the heat exchanging efficiency. The fundamental fluid structure of HAR is the Jet In Cross Flow (JICF), which is common in environmental flows, e.g., heat dispersions into the atmosphere. Many numerical analyses have been performed for JICF using incompressible CFD models that rely on the Boussinesq approximation for buoyancy force consideration. For predictions of HAR in actual atmospheric conditions, it is desirable to use meteorological models that compute unsteady compressible flows (Large Eddy Simulation based on compressible fluid equations, compressible LES). This study presents numerical simulations of JICF using a compressible LES, firstly to confirm the reliability of compressible LES and secondly to investigate the validity of the Boussinesq approximation, which is used in incompressible models, in JICF simulations. The present compressible LES results were compared with those from other incompressible CFD models that employed the same equally spaced grid settings. The comparison has confirmed the reliability of the present compressible LES. It has been also confirmed that the present compressible LES model reproduces the typical vortex structures of JICF.

When calculating the transport of heat by using incompressible models, the Boussinesq approximation is usually employed to consider the buoyancy due to hot air. The approximation is not, however, applicable to large temperature differences between hot air and ambient air. The compressible LES model, which is free from such approximation, can provide a reference for the incompressible models. The present compressible LES model was applied to the case of JICF with hot air, i.e., high temperatures. The obtained reference data has revealed the applicability limits of the Bousinessq approximation.

It is expected that the present results will advance the understanding and the prediction of exhaust heat diffusion phenomena under realistic weather conditions with unsteady winds in the future.

Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A STUDY OF CONTINUUM-SCALE STRESS CALCULATION ON FINITE ELEMENT METHOD INDUCED BY MOLECULAR-SCALE STRUCTURAL TRANSITION

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ABSTRACT

In this study, we develop a methodology to couple molecular-scale thermodynamic properties, derived from molecular dynamics (MD) simulations, with the continuum-scale finite element method (FEM). Typically with the FEM approach, single-phase constitutive equations are determined a priori to define the stress-strain relationship. However, polymers and gas hydrates, which may undergo structural changes and phase transitions, have multiple stress-strain responses that are condition-dependent. In previous research, it has been observed that polycarbonate exhibits a unique drop in structural resistance with increased void generation. Carbon dioxide hydrate has different mechanical resistances for tensile and shear modes. These features can only be examined using MD simulations, which accurately capture the stress-strain relationships at each stage of the deformation process. To capture these properties and, in turn, determine their relation to continuum-scale stress fields, we utilized MD simulations as a replacement for specific constitutive equations in the FEM scheme. To begin with, we propose a fully coupled FEM-MD approach. For the FEM scheme, we utilized a work conjugate of the first Piola Kirchhoff Stress tensor and the deformation gradient. This allows us to incorporate the non-linear region of the stress-strain relationship. The update of the displacement is performed by explicit time integration with the central difference scheme. Then, the deformation gradient tensor is calculated at each integration point and applied to the boundary conditions of the representative unit-cell (r-cell) in the MD simulation. For MD simulations, a certain amount of time is required for equilibration and potential energy minimization. Here, we used a Nose-Hoover thermostat to maintain the r-cell's temperature. From the equilibrated r-cell, we obtain the Cauchy stress tensor and use it as a substitute for the internal force in the FEM scheme. Subsequently, we compare the results of fully coupled FEM-MD with one-way coupled FEM-MD, which we developed previously. Since the one-way coupled approach does not receive feedback from MD, continuum-element deformation is determined only from FEM calculations. On the other hand, in the fully coupled approach, there is an interplay between the continuum and molecular scales which results in relaxing the stress-strain response. In the future, we plan to establish a methodology to fully capture the relationship between molecular-scale structural stability and deformation history at the continuum-scale of the material.

Towards predictive digital twins: Innovative algorithms for physics-, data-assisted and hybrid modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A DIGITAL TWIN FRAMEWORK FOR CIVIL ENGINEERING STRUCTURES

Matteo Torzoni[1], Marco Tezzele[2], Stefano Mariani[1], Andrea Manzoni[1] and Karen Willcox[2]*

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ABSTRACT

In this talk, I will present a digital twin (DT) formulation for the structural health monitoring of civil engineering structures [1], with a focus on bridges.
A DT is a virtualization of a physical asset built upon a set of computational models that dynamically update to persistently mirror a unique asset of interest throughout its operational lifespan, enabling informed decisions that realize value.
The talk covers the health monitoring, predictive maintenance, and management planning of civil structures. The asset-twin coupled dynamical system is encoded using a probabilistic graphical model (PGM) [2] which provides a general framework for data assimilation, state estimation, prediction, planning, and learning while accounting for the associated uncertainty. The assimilation of high-dimensional multivariate time series describing the vibration response is carried out by exploiting physics-based reduced order methods and deep learning models. The numerical models allow automated selection and extraction of optimized damage-sensitive features and real-time assessment of the structural state of a bridge.

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Machine learning for large scale models in physics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPLORING RIEMANN SOLVERS, MACHINE LEARNING SURROGATES, AND SHOCK TRACKING IN HYPERBOLIC PDE SYSTEMS

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ABSTRACT

In the computational modeling of systems governed by hyperbolic partial differential equations (PDEs), Riemann solvers (RS) assume a pivotal role. The landscape of available Riemann solvers encompasses various options, each characterized by distinct merits and drawbacks related to accuracy, computational efficiency, and cost. Preeminent among these solvers is the exact RS, acknowledged for its superior accuracy; however, its implementation is intricate and computationally demanding. Conversely, the Roe solver and the Harten, Lax, and Van-Leer (HLL) solver offer simplicity and computational efficiency, yet the former falters in addressing strong shocks and contact discontinuities, while the latter tends to yield excessively diffusive solutions and struggles with intricate wave structures. Both solvers also grapple with challenges in handling transonic rarefactions, and the Roe solver lacks positivity preservation. Modifications, such as entropy fixes for Roe or the HLL with Contact solver, may enhance accuracy selectively but lack universality. Concurrently, the application of machine learning, particularly deep learning, has witnessed a notable surge in the field of mechanics. Consequently, the integration of deep neural networks (DNNs) as surrogates for exact RSs has gained attention, offering cost-effective approximations while preserving critical attributes like resilience in the face of strong shocks or transonic rarefactions. This study endeavors to craft a DNN-based surrogate endowed with additional properties, including hyperbolicity, conservation, and consistency, through the assimilation of concepts from the burgeoning field of differentiable programming. Furthermore, our objective is to harness this surrogate in the domain of shock tracking, a field experiencing renewed interest, characterized by frequent encounters with strong shocks and intermittent confrontations with transonic rarefactions.

Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A SMOOTH YIELD PLASTICITY THEORY FOR MODELING FATIGUE IN METALS: THEORY, COMPUTATIONS AND EXPERIMENTAL VERIFICATION

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ABSTRACT

Fatigue is one of the most studied and modeled phenomena in engineering practice due to its practical importance. In this talk, we describe a novel smooth yield rate-independent J2 plasticity-based constitutive theory for modeling plastic deformation in metals [1], and its efficacy is demonstrated by the accurate prediction of low-cycle to high-cycle fatigue life in a variety of metallic alloys (aluminum, steel etc.) even under variable amplitude loading conditions [2]. The key aspect to our theoretical approach is that we are able to accurately track the hysteresis caused by micro-plastic deformation which occurs under fatigue loading, and this is the physical cause for fatigue-accumulated damage in metallic materials. We have also computationally-implemented the smooth yield plasticity-based constitutive model into the implicit-based ABAQUS/Standard finite-element program through a UMAT subroutine interface [3], and the numerical implementation of the constitutive theory into a finite-element framework is shown to be robust.

Traditionally, the material parameters responsible for the estimation of fatigue life are determined through a series of low-cycle to high-cycle fatigue experiments e.g. through a unified Coffin-Manson and Basquin approach. However, in our approach, material parameters in the constitutive theory were calibrated to a single uniaxial and cyclic loading simple compression experiment, and a single low-cycle fatigue experiment (less than a few hundred cycles). With the constitutive parameters calibrated, we are then able to independently and accurately predict a variety of fatigue experiments from low-cycle to high-cycle loading conditions under uniaxial (cyclic tension-compression) and multi-axial loading conditions (axial-torsional under proportional or non-proportional loading) through a series of finite-element simulations [3]. Finally, another main contribution of the present work is that our developed theoretical and computational framework for modeling uniaxial and multi-axial low-cycle and high-cycle fatigue loading in metals is able to provide a better prediction for fatigue life estimation compared to several other popular fatigue life prediction-based models in the literature.

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Biomechanics of hard tissues: From experiments and simulations to clinical applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREDICTION OF PATIENT-SPECIFIC KNEE JOINT DYNAMICS IN TIBIAL FRACTURES

Elin Theilen[*1], Anna Rörich[1], Joachim Georgii[1] and Kaywan Izadpanah[2]*

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ABSTRACT

Introduction
The knee joint is one of the most complex human joints and fracture or morphology of the human femur and / or tibia are among the most common in the event of osteoporosis or injuries. Since the tibia supports a great amount of body weight, it plays an important role in maintaining the stability and functionality of the knee joint. Understanding the importance of tibia fractures in knee dynamic analysis is crucial not only for assessing the extent of the injury but also for predicting critical dynamical motion and making informed decisions about the necessity of surgery. Models that take into account the patient-specific knee joint motion are supposed to largely improve surgery planning and outcome. State-of-the-art finite element (FE) knee joint models are highly complex, computationally demanding and time-intensive.

Methods and results
We propose a simplified knee joint model based on position-based dynamics (PBD) for real-time prediction of patient-individual knee joint motion [1]. The PBD-model was successfully verified against to the state-of-the-art FE model [2] in dynamic knee motion. Magnetic resonance (MR) images of human knees were obtained in a study of eleven healthy volunteers, which was approved by the ethics committee of the Albert-Ludwigs University Freiburg (Nr. 91/19 – 210696, 19 August 2021). We compared two motion sequences going from 0° knee flexion to 20° flexion and adding 1) internal or 2) external rotation torque [3]. The PBD model predicts similar motion while being approximately 150-times faster.

To analyse fracture defects, we additionally consider different artificial tibial fractures in the dynamic analysis to understand critical impacts on knee joint motions and derive whether treatment is necessary. We believe that PBD prediction yields a good trade-off between accuracy and time constraints and thus, is able to efficiently support the clinical workflow.

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Data-driven device and circuits models
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HAMMERSTEIN-WIENER DATA-DRIVEN COMPACT CIRCUIT MODELING. PART 2: EXTENSION TO MULTIPLE LOADS AND FREQUENCY DOMAIN TRAINING

Ethan Thieme[*1], Biliana Paskaleva[2], Xu Chen[1], Pavel Bochev[2], Joshua Hanson[1], Paul Kuberry[2] and Ian Wilcox[2]*

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ABSTRACT

In Part 1 we demonstrated that Hammerstein-Wiener (HW) models are an effective tool for modeling a circuit's behavior, especially when the behavior can be easily separated into a nonlinear, DC, portion and a linear, AC, portion, such as in, e.g., amplifier circuits. In this talk we shall focus on the development of such models for a simple differential amplifier with particular emphasis on effects that depend on the frequency of the input signal. Specifically, differential amplifiers exhibit gain degradation and phase shift as this frequency increases. Capturing this behavior in the time domain requires training data spanning a wide range of frequencies and can lead to very large training datasets.

In this talk we show that training the linear time invariant (LTI) block of the HW model in the frequency domain is an effective alternative to training in the time-domain data that leads to significant reduction in the size of the necessary data sets. In particular, the training process reduces to a regression of a rational function (the transfer function) from frequency domain data. Once this function is fitted, it is trivial to convert the model back to the time domain thereby enabling conventional Spice time-domain simulations.

Lastly, for the HW model to be useful in numerous situations, it has to be generalized to operate for different loads at its output. To that end we fix the structure of the rational function representing the transfer function and treat its coefficients as functions of the load. Given a desired load range for the circuit simulation we then sample this range at a finite set of loads and learn the coefficients corresponding to each load value. To simulate the circuit at a specific load value in the desired range we use interpolation between these predetermined coefficients to construct a transfer function corresponding to the specified load value. Again, this function can be easily converted from the frequency domain to the time domain to perform conventional Spice simulations.

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Emerging topology and shape optimization techniques in computational design of materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INVERSE DESIGN OF PERIODIC MICROSTRUCTURES WITH TARGETED NONLINEAR MECHANICAL BEHAVIOUR

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ABSTRACT

Structural metamaterials derive their mechanical properties from the distribution of material on the microscale, typically in the form of discrete microstructure geometries, rather than the properties given by the bulk material. Interest in structural metamaterials has greatly accelerated with the increased adoption of additive manufacturing (AM) technologies. Metamaterials offer the possibility of designing materials with highly tailored, application specific properties. This work introduces an inverse design framework for the precise tailoring of desired nonlinear mechanical responses in periodic microstructures, with particular focus on prescribed nonlinear stress-strain relationships. The topology optimization hinges on minimizing the error between the target and realized properties of the microstructures, using a deformation-driven homogenization framework. The periodic constraints needed for the microscale equilibrium equation are imposed through strongly enforced periodic boundary conditions and the removal of the translational nullspace, avoiding the need for Lagrange multipliers, greatly simplifying the implementation. To further aid the design of discrete designs an intermediate density penalty constraint is proposed.

Two main contributions are made to the state-of-art in this field:
1) A effective framework for designing periodic microstructures with targeted nonlinear stress-strain relationships is developed;
2) An intermediate density penalty constraint formulation is presented to encourage the formation of discrete microstructure designs and further aid the optimization convergence.

Using a materially linear but geometrically nonlinear hyperelastic model, a deformation-driven homogenization approach is utilised to derive the homogenized quantities required for the optimization. Several numerical examples are tackled to demonstrate the efficacy of the framework. We demonstrate that the framework is able to design microstructures that accurately replicate the targeted stress-strain relationships with less than 10% errors. The IDP constraint is also shown to encourage the formation of discrete microstructure topologies with less than 2% grey material in all designs. As discrete designs better promote nonlinear behaviours, the IDP constraint further aids the optimization convergence. Finally, the effect of initialisation is also studied.

This framework lays the foundation for multiscale nonlinear optimization, where nonlinear structures are optimized on the microscale (either concurrently or in a offline manner) to design nonlinear macroscale structures with highly nonlinear structural responses. For example, the design of deployable nonlinear structures which exhibit bi-stable behaviours and or deploy at targeted loads.

Constitutive modeling of complex materials with machine learning and artificial intelligence
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NOVEL DIFFUSION TENSOR BASED MYOCARDIAL MATERIAL MODEL: FORM DETERMINATION USING NEURAL NETWORKS

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ABSTRACT

Cardiac tissue has a very complex structure that induces substantial local mechanical anisotropy that varies with anatomical location and in various pathologies. Structural information for cardiac tissue is readily available using Diffusion Tensor Magnetic Resonance Imaging. Interestingly, to date only the eigenvectors of the diffusion tensor D have been used to determine the local fiber direction in myocardial material models. Yet, D contains much more tissue structural information. In the present study, we developed a novel method to directly incorporate D into the material model, allowing for locally heterogenous anisotropic mechanical behaviors within each test specimen. To quantify the unknown form of the material model, we introduced a neural network to represent the strain energy function following [1]. In this approach automatic differentiation tools are utilized to streamline computations. This approach allows for generalized model form determination directly from the experimental data. This is a very important step as form determination for hyperelastic biological tissues remains a major hurdle in accurate simulation of disease and surgical planning.

The inverse model framework starts by acquiring force-displacement pairs from the experimental data. A generic form was provided to the inverse model containing the pseudo-invariants I4 and I5. A JAX-FEM solution was found where the material is modeled as nearly incompressible. The parameters are then trained by minimizing the error between the force data and the prediction of the model. The gradients were obtained from the JAX-FEM solver through automatic differentiation. During training, if parameters fall to zero, it shows terms disappearing from the final form.

The method was first tested on the Li model [2], which was used to fit highly anisotropic myocardial data using the eigenvectors of D. This dataset contains 5 specimens tested under various protocols. Based on the results of the new form, we developed form for the directional strain energy using exponential forms of I4 and I5. To allow for local heterogeneity, D was incorporated as a weighting distribution. We note that tension/compression differentiation was also required, unique to modeling. The final form obtained an excellent fit to the data with only three material constants. The incorporation of D gives the material model more structural information making the final form much simpler, as well as allowing for regional heterogeneity. Next steps include incorporation into full 3D cardiac models.

[1] Linke et al., Acta Biomaterialia, 160:134-151(2023)
[2] Li, DS et al., J Mech Behav Biomed Mater(2020), 103, 10350

Computational modeling of extreme-loading events
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING OF HIGH DEFORMATION LAGRANGIAN BLAST MECHANICS USING ISOGEOMTRIC ANALYSIS AND AN IMMERSED DOMAIN METHOD

Michael Scott[1], Derek Thomas[1], Greg Vernon[1], Stephen Beissel[2] and Charles Gerlach[2]*

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ABSTRACT

This work presents a comprehensive exploration of the implementation of smooth spline shape functions and the immersed finite cell method for the simulation of high deformation Lagrangian mechanics in blast scenarios. The focus is on demonstrating computational efficiency and robustness through the utilization of these techniques. The implementation of the finite cell method is discussed in detail, supported by specific examples showcasing its effectiveness.

The study incorporates Cook's membrane to elucidate how the integration of smooth spline shape functions, finite cell method, and reduced quadrature methods can mitigate material locking issues. Plastic deformation is analyzed through Taylor impact simulations, providing insights into the behavior of materials under high-deformation conditions.

To assess the capability of the proposed methods in wave propagation, the Hopkinson bar is employed. The results illustrate that smooth splines and an immersed mesh can accurately approximate the mechanics of waves propagation.

Furthermore, the study explores diverse scenarios, including example penetrators, self-contact situations, and the buckling of a square tube. Each scenario serves to highlight the versatility and applicability of the implemented techniques in a number of common situations.

In conclusion, the presented work not only details the implementation of smooth spline shape functions and the finite cell method but also demonstrates their efficacy through a series of simulations. The findings in this work contribute to the advancement of automated computational methods for accurately and efficiently modeling complex high-deformation scenarios in Lagrangian mechanics.

Coupled computational mechanics: Solutions for FSI simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INTERFACE MECHANICS FOR EXPLICIT EULERIAN TO EXPLICIT LAGRANGIAN COUPLING USING THE MODIFIED IMMERSED FINITE ELEMENT METHOD

Jesse Thomas[*1], Scott Miller[1], Chad Hovey[1], Matthew Mosby[1], Jennifer Rees[1], Michael Wong[1], Anthony Agelastos[1], Mark Christon[1], David Hensinger[1] and Benjamin Treweek[1]*

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ABSTRACT

The modified Immersed Finite Element Method (mIFEM) [1] is an overlapping mesh method that couples a Lagrangian foreground solution with an Eulerian background solution. Coupled analysis techniques like the mIFEM can be used to model crash or impact/penetration scenarios, combining a Lagrangian mechanical system model with an Eulerian model of the material being impacted. These classes of problems often involve extensive contact, and the mechanics between material surfaces (e.g., bonding, frictionless sliding, Coulomb friction, nonlinear pressure dependent friction) can strongly influence the response of systems. We explore formulations of interface mechanics between Lagrangian surfaces and Eulerian materials using the mIFEM. We present the mIFEM coupling method and numerically investigate contact formulations on a set of exemplar problems. Accuracy will be assessed against canonical contact and impact cases, and the favored formulation is demonstrated with a realistic example problem.

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[1] Xingshi Wang, Lucy T. Zhang, Modified immersed finite element method for fully-coupled fluid–structure interactions, Comput. Methods Appl. Mech. Engrg. 267 (2013) 150–169.

Multi-scale, multi-rate damage and fracture: Models, experiments, and simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADIABATIC SHEAR BAND MODELLING IN TI6AL4V USING FINITE ELEMENT APPROACHES

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ABSTRACT

Ti6Al4V is an alloy which is widely used in industry due to it having a number of desirable properties, including its high strength to density ratio. However, the material is highly susceptible to failure via the adiabatic shear banding mechanism. Whilst there exists a large sum of simulation work in the literature on the topic, appropriate methods for the meshing and treatment of the material heterogeneity, which influences the processes of shear band initiation and development, remains an active area of research.

The present study utilises 3D finite element hydrocodes to assess the modelling sensitivities in simulations of spontaneous shear band formation, using the thick-walled cylinder experimental geometry. To capture the effect of material heterogeneity, a Lagrangian perturbation field is applied to the yield strength, inducing localisation in the target material.

Data-driven device and circuits models
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CHALLENGES AND APPROACHES FOR REINTEGRATING REDUCED-ORDER MODELS IN CIRCUIT SIMULATION

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ABSTRACT

Reduced-order modeling has been an active area of research for several decades, focusing on the creation of efficient and accurate approximations for computationally expensive mathematical models. For circuit simulation, reduced-order models have been extensively studied for large interconnect networks that are often embedded in larger VLSI (Very Large Scale Integrated) circuit designs. For nonlinear and linear time-varying circuits, methods have also been considerably explored, but to a lesser extent than their linear time-invariant (LTI) counterparts. This presentation will focus on what is rarely addressed in literature, the practical aspects of reintegrating reduced-order models into a larger circuit design. The discussion will illustrate challenges and demonstrate viable approaches for implementing a modular design flow that includes reduced-order models using Xyce [1].

Xyce is an open source, SPICE-compatible, high-performance analog circuit simulator that provides both time and frequency domain analysis capabilities. Internal to Xyce there are methods for reducing LTI circuits based on moment-matching approaches, like the Passive Reduced-Order Interconnect Macromodeling Algorithm (PRIMA) [2]. This algorithm will be used as an exemplar to explore the challenges of reintegrating reduced-order models into a modular design flow and illustrate approaches, like sparsification [3], that can help reduce total simulation time. Approaches for reintegrating reduced-order models developed external to Xyce will also be discussed.

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[2] Odabasioglu, A., Celik, M., & Pileggi, L. T. (2003). PRIMA: Passive reduced-order interconnect macromodeling algorithm. The Best of ICCAD: 20 Years of Excellence in Computer-Aided Design, 433-450.
[3] Matsumoto, Y., Tanji, Y., & Tanaka, M. (2001). Efficient SPICE-netlist representation of reduced-order interconnect model. In Proceedings of ECCTD (Vol. 2, pp. 145-148).

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Contact and interface mechanics: Modeling and computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IGA-BASED MODELLING OF WET GRINDING PROCESSES WITH SPECIAL FOCUS ON HYDRODYNAMIC PROPERTIES

Paul Thunich[*1], Yan Tong[1], Michael Müller[1], Oliver Schömig[12], Robar Arafat[12] and Christoph Herrmann[12]*

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ABSTRACT

In grinding processes, process parameters are usually set based on experience or empirical trial-and-error tests, as there is limited knowledge about basic interactions. Especially in the development of new cutting fluids, a conflict arises between cooling effects and hydrodynamic load-bearing effects. Therefore, a model should be developed, in order to investigate interactions and optimize wet grinding processes.

Besides this hydrodynamic conflict, further processes and properties determine the wet grinding process. These include the contact mechanics of the grain-workpiece interface, the temperature distribution, the temperature rise due to friction and fluidic friction and the associated viscosity decrease, the grinding wheel structure, as well as abrasion and deformation effects and even the cutting fluid supply strategy, all of which more or less influence the grinding performance. Therefore, it is generally challenging to develop a model which considers all subprocesses and properties to a satisfactory level for wet grinding.

With a special focus on the cutting fluids in grinding, this paper presents a hydrodynamic analysis of the process, which is done by using the Reynolds equation and NURBS-based isogeometric analysis (NURBS-IGA). In combination with a mortar-based cavitation algorithm and the heat equation, a model within the NURBS-IGA framework is built that enables the contact properties to be modelled within reasonable time. The results generated by the model correspond to modelling results from commercial CFD tools such as Ansys Fluent with good accuracy. In this context, the necessary stabilization techniques need to be mentioned, necessitated by the convection-dominated governing equations and the small number of computational nodes in the NURBS-IGA. Additionally, it can be shown to what extent the consideration of dependencies of the material properties of the fluids is necessary and in which cases they can be neglected to decrease the computational cost. The resulting model is a performant description of the hydrodynamic effects, which is easily applicable to other cases like lubricated journal bearing calculations and that is also validated via experimental measurements.

Finally, to model the entire wet grinding process, the model is combined with other influencing factors in the further course. These include the consideration of the grinding wheel porosity, which reduces the maximum hydrodynamic pressure generated, the material removal and further influences, all within the framework of NURBS-IGA.

In this way, the model is a valuable basic approach and has a large potential for construction of complex models and even iterative optimizations in the field of wet grinding.

The phase field method for fracture: Theory, numerics, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FRACTURE PATTERNS AND DYNAMICS OF SOFT MATERIALS□PHASE FIELD MODELING

*Fucheng Tian**[1]

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ABSTRACT

Soft materials possess unique traits of withstanding large strains and exhibiting high recoverability, rendering them irreplaceable in cutting-edge fields such as life sciences and soft robotics. Understanding the complicated fracture behavior of such materials is not only of urgent application demands but also a longstanding pursuit in interdisciplinary fundamental research, spanning the realms of materials science, physics, and nonlinear mechanics. A well-grounded theoretical framework has been established to date for fracture in linear elastic regimes. However, the fracture in soft materials typically involves nonlinearities associated with large strains, exhibits diverse dynamic morphologies, involving straight, oscillation, branching, and supershear fracture. These intricate crack dynamics are believed to be associated with nonlinearity. Using the latest developed dynamic phase-field model, we successfully reproduce various crack morphologies and establish crack stability phase diagrams for three distinct soft materials. The contrasting phase diagrams highlight the crucial role of nonlinearity in regulating crack dynamics. In strain-softening materials, crack branching prevails, limiting the cracks to sub-Rayleigh states. Yet strain-stiffening stabilizes crack propagation, allowing for the presence of supershear fracture. Of particular interest is the large-strain linear elastic materials, where crack oscillation is readily triggered. Moreover, our findings suggest that the increase in characteristic wave speed due to strain-stiffening can account for the observed transition of cracks from sub-Rayleigh to supershear regimes.

Microstructures of chemically complex materials and their impacts on material properties from multiscale simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPLORING MECHANICS AND PIEZOELECTRIC PROPERTIES VIA MULTI-SCALE SIMULATIONS IN DEFECT-ENGINEERED ZINC INDIUM SULFIDE (ZIS) FOR PHOTOCATALYTIC WATER SPLITTING

Ming-Yuan Hung[1], Yen-Ting Kuo[1], Jih-Jen Wu[1] and Hong-Kang Tian[1]*

[1]National Cheng Kung University

ABSTRACT

This study delves into the realm of chemically complex materials, focusing on Zinc Indium Sulfide (ZnIn2S4, ZIS) for efficient photocatalytic water splitting into hydrogen (H2) and oxygen (H2). Recognizing the pivotal role of microstructures in chemically complex materials, our research emphasizes the impact of defects in ZIS, a material with multiple principal chemical components, on its H2 production efficiency. We explore the optimization of material defects, particularly sulfur (S) and indium (In) vacancies, under external stress to enhance H2 production through dipole and piezoelectric effects. To unravel the intricate process-structure-property relationships in ZIS, we utilize a multi-scale computational approach. Density Functional Theory (DFT) is employed to calculate dipole moment, dielectric, elastic, and piezoelectric properties under varying defect compositions. These properties are then integrated into a continuum model developed through Finite Element Analysis (FEA), bridging mechanical and electrical phenomena to simulate the electric potential distribution (voltage) in both pristine and defective ZIS. Our simulations demonstrate a marked increase in voltage, induced by internal dipole moments and piezoelectric effects, especially pronounced along the (100) and (010) crystal orientations in defective ZIS. This enhanced voltage leads to improved charge separation, substantially increasing the H2 production rate upon electron excitation and generation of electron/hole pairs. Our findings contribute vital insights into the microstructural influences on the photocatalytic performance of ZIS, offering design principles for advanced materials in renewable energy applications. This study exemplifies the power of computational techniques in elucidating the complex interplay between microstructure and properties in chemically complex materials, aligning with the core focus of this symposium.

Buckling analysis and design of thin-walled structures based on novel and intelligent computational methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DIGITAL TWIN FOR STRUCTURAL LOAD-CARRYING CAPACITY MONITORING AND PREDICTION

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ABSTRACT

The digital twin method is proposed for the structural load-carrying capacity monitoring and prediction of complex shells. Firstly, a multi-source data fusion approach is introduced to integrate simulation data with sensor readings, enabling the construction of a high-accuracy and robust digital twin. Secondly, an optimal sensor placement strategy is established for complex curved structures, enhancing the monitoring efficiency of sparse sensors. Thirdly, a dynamic update method for the digital twin is developed based on a reduced order model, ensuring the accuracy and reliability of the digital twin in practical strength assessment scenarios that account for deviations. Finally, the proposed method's effectiveness is validated through structural strength tests on open hole panels, hierarchical stiffened plates, and cargo spacecraft cabins. The results demonstrate that the method can achieve real-time and high-accuracy structural load-carrying capacity monitoring and prediction of complex shells.

Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PERIODIC LAGRANGIAN ANALYSIS WITH MESH RECONSTRUCTION FOR OFFSHORE GEOTECHNICAL LARGE DEFORMATION PROBLEMS

Ran Tu[1], Huan Zhao[2], Shubhrajit Maitra[1] and Yinghui Tian[*1]*

[1]The University of Melbourne
[2]Tianjin University

ABSTRACT

Large deformation process is commonly encountered in offshore geotechnical applications, with typical examples including penetrometer penetration, anchor installation (keying), spudcan preloading and pipeline laying and buckling. Numerical large deformation modelling still remains one of the most challenging aspects of computational geomechanics. Offshore engineers require reliable and accessible numerical approaches to simulate large deformation processes. The traditional Lagrangian finite element analysis is inadequate due to excessive mesh distortion. An efficient approach, Periodic Lagrangian Analysis with Mesh Reconstruction, is proposed to overcome the numerical difficulties. This paper first offers a narrative of currently available large deformation modelling approaches within the space of offshore geotechnics. Periodic Lagrangian Analysis with Mesh Reconstruction is then proposed with clear demonstration of concept and implementation. The performance of the proposed approach is demonstrated by showcasing some of its applications to model: (a) anchor trajectory during installation of plate anchor; (b) penetration of conical footings; and (c) spudcan penetration next to an existing footprint.

Advanced materials: Computational analysis of properties and performance
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FIRST-PRINCIPLES STUDY ON THE STRUCTURAL AND ELECTRONIC PROPERTIES OF ADVANCED TWO-DIMENSIONAL MATERIALS

Yujia Tian[12], Devesh Kripalani[1], Ming Xue[2], Swee Lee Gan[2], Shaofan Li[3] and Kun Zhou[1]*

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ABSTRACT

Ever since the successful isolation of graphene in 2004, two-dimensional (2D) materials have garnered much attention due to their vast possibilities of property tuning, making them promising candidates for various applications in next-generation electronics. Employing first-principles calculations, we perform a series of studies examining the nuances of tuning the structural and electronic properties of 2D materials, providing insights into the novel design of related devices.

A prevalent approach to property modulation is strain engineering. However, rippling—a consequence of the intrinsic instability in free-standing 2D sheets—becomes prominent, especially during in-plane compression. In the literature, this rippling phenomenon has been proven to have a contrasting, remarkable impact on the properties of different 2D materials. Using antimonene as a case study, we demonstrate a systematic way of examining the effects of rippling by comparing the flat and rippled structures under uniaxial in-plane compression, and the underlying mechanism is scrutinized. Rippled antimonene is shown to exhibit highly stable properties like the work function and band gap upon structural relaxation at a range of compression levels, closely resembling its pristine state. Conversely, various changes are observed in its flat counterparts. The identification of optimal ripple amplitudes under strain for which the electronic properties of the pristine condition can be recovered will be highly significant in guiding the rational design of antimonene-based devices.

Further, we delve into the impact of out-of-plane compression. Fermi level pinning (FLP) at metal–2D semiconductor contact can hinder the tuning efficacy. We perform a detailed investigation of contact systems formed by common electrode materials and 2D tin monoxide (SnO), a promising transistor channel material. By analyzing the geometry, bonding strength, charge transfer and tunnel barriers of charges, and electronic properties, we unearth the mechanisms behind FLP. We also propose the insertion of a graphene buffer layer at the contact, which efficiently alleviates the metal-induced gap states and enhances the tunning efficiency of out-of-plane compression. This work scrutinizes the possibilities of employing monolayer SnO in field effect transistors by systematically examining its contact with various electrode materials and methods of property tuning. The established model can be modified in the future to accommodate other factors to assess their impacts on the contact performance.

Advanced materials: Computational analysis of properties and performance
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING HARDENING AND DAMAGE EVOLUTION IN ADDITIVELY MANUFACTURED METAL MATRIX COMPOSITES USING A LARGE-STRAIN ELASTO-VISCOPLASTIC FFT-FRAMEWORK

Claire Ticknor[*1], Jamila Khanfri[2], Alex Butler[2], Joshua Kacher[2], Aaron Stebner[2] and Ashley Spear[1]*

[1]*The University of Utah*
[2]*Georgia Institute of Technology*

ABSTRACT

Particle-reinforced metal matrix composites (MMCs) are composed of ceramic particles in a metal alloy matrix. The toughness and light weight of the ductile metal matrix in concert with the stiffness and strength of the ceramic reinforcement are exploited to enhance properties—such as the tensile strength, fatigue strength, high-temperature stability, wear resistance, thermal shock resistance, and general functionality—relative to the individual constituents. Conventional manufacturing of MMCs by casting or powder metallurgy has limited production to parts with simple geometries that are expensive with high lead and machining times. However, the use of additive manufacturing (AM) has enabled components to be made with high geometric complexity and customization, and rapid prototyping with a lower cost. Specifically, laser powder bed fusion (LPBF) produces geometrically complex MMC structures with easily adjustable amounts of reinforcement particles, attractive strength and weight characteristics, and desirable microstructure characteristics such as small grain sizes and more equiaxed grain shapes, all influenced by manufacturing parameters and composition. Optimization of MMC properties and parameters done experimentally requires large amounts of time and resources to produce powders of varying compositions, print high quality parts using LPBF, and analyze the physical and mechanical properties. Thereby, to achieve tailorable designs of MMCs that efficiently meet specific mechanical performance targets requires high-fidelity models that accurately capture the effects on the hardening and damage evolution of the MMC.

In this work, we propose a modeling framework based on a large-strain elasto-viscoplastic fast Fourier transform (FFT) code, in which we incorporate a work-hardening formulation coupled with triaxiality-based continuum damage mechanics to model the hardening and damage evolution of MMC material as a function of particle reinforcement composition. While most models of MMCs focus on one or two hardening mechanisms for a specific composition, our proposed model considers several hardening mechanisms specific to both MMCs and the AM process while accounting for the effects of reinforcement particle composition. The main hardening mechanisms considered are geometrical differences between the metal matrix and the spherical particle, differences in thermal expansion exasperated by the AM process, differences in hardness between the metal matrix and the ceramic particles and increases in grain boundary abundance compared to the pure matrix material. The superposition of hardening mechanisms, efficacy of the framework, and inspection of fracture-initiation-to-microstructure-neighborhood relationships will be presented. The framework will make the task of exploring the high-dimensional design space for polycrystalline MMCs by AM tractable.

Mechanobiology of cells, vesicles and biomembranes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTER SIMULATIONS OF LIPID NANOPARTICLES FOR DRUG DELIVERY

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ABSTRACT

Molecular dynamics simulations use detailed models based on atomistic or near-atomistic resolution to simulate the properties of biomolecular systems. Lipid nanoparticles are the technology used to deliver mRNA vaccines and have broad potential for drug and gene delivery in general. A key ingredient in these formulations is cationic lipids that change protonation state during processing in endosomes inside the cell before their cargo is released. We have simulated the properties of these cationic lipids in several contexts relevant for drug uptake and release through local remodeling of lipid nanoparticles and endosomal membranes. We are attempting to link these to the efficacy of mRNA release.

Physical models and reduced order models augmentation with data for physics-informed machine learning in real-world applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THERMODYNAMICS INFORMED GRAPH NEURAL NETWORKS FOR DOMAIN DEPENDENT PROBLEMS

Alicia Tierz[1], Icíar Alfaro[1], David González[1], Francisco Chinesta[2] and Elías Cueto[1]*

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ABSTRACT

Currently, Computational Fluid Dynamics (CFD) and Solid Mechanics (CSM) tools deliver precise simulations, enabling companies to save substantial resources in comparison to traditional methods. However, a significant drawback lies in the extensive CPU time required for a single simulation. This computational cost escalation is due to the complex physics inherent in these models and the necessity for a large mesh size to analyze intricate geometries. To mitigate this prolonged processing time, Deep Learning (DL) is being harnessed to address the issue, yielding real-time results with minimal compromise on accuracy.

Presented here is a DL approach aimed at predicting various scenario specifics within specific domains, such as fluid movement in a glass or the behavior of a viscoelastic beam. We advocate for the incorporation of both geometric and thermodynamic data to refine the precision and adaptability of the resulting integration approach. To harness information derived from the Lagrangian portrayal of movement, we will employ graph neural networks (GNNs) [1]. The application of geometric deep learning reduces data consumption due to inherent symmetries in the problem.

The architecture is meticulously designed to learn the GENERIC (General Equation for Non-Equilibrium Reversible Irreversible Coupling) [2] structure of the problem, an extension of the Hamiltonian formalism used for modeling broader non-conservative dynamics.

The employed architecture is rooted in Thermodynamics Informed graph neural networks [3]. A comprehensive database is constructed using a CFD tool, utilized to train the graph-based structure. The network undergoes testing across various geometries and materials. In addition, the model will be tested with never-before-seen physical conditions to verify that it is capable of generalizing physical behavior well.

Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MODIFIED INHERENT STRAIN MODELING FRAMEWORK FOR PREDICTING RECOATER INTERFERENCE IN LASER POWDER BED FUSION

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[1]University of Pittsburgh

ABSTRACT

Preventing recoater interference and crash is essential in laser powder bed fusion (L-PBF) process for printing parts with overhangs. These issues may compromise product quality by increasing surface roughness, reducing dimensional accuracy, and introducing defects into the parts. This work proposes an integrated simulation and experimental framework to predict potential recoater interference for a given part designed for L-PBF fabrication. In this framework, the criterion for recoater interference is defined to occur when the deformation of the part in the build direction exceeds the thickness of a newly spread powder layer after recoating. The largest deformation in the build direction is assumed to occur at the edge of a part and is postulated to be the sum of two contributions: global thermal deformation and local edge deformation. The global thermal deformation, generated by relaxation of the thermal stresses induced by the rapid laser melting and solidification over the entire part, is predicted using the modified inherent strain (MIS) method. A key novelty in this work lies in employing location-dependent inherent strains (ISs) in the MIS method to simulate the global thermal deformation of overhangs, which shows 60% improvement in prediction accuracy compared with that using constant ISs. On the other hand, the local edge deformation, associated with the melt pool dynamics and deformation near the edge, is estimated by reconciling the MIS simulated and experimentally measured deformation on several overhang wedges. The validity of the proposed framework for predicting recoater interference is confirmed by experiments on different part geometries with overhangs.

Imaging-based methods in computational medicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTATIONAL MODELLING AND OPTIMIZATION OF LEPTOMENINGEAL ANASTOMOSES CONFIGURATION: A PATIENT-SPECIFIC APPROACH USING 4D FLOW MRI AND SPECT

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ABSTRACT

Leptomeningeal anastomoses (LMAs) are arteries connecting otherwise terminal vasculature territories on the cerebral cortex. They aid ischemic stroke recovery by restoring blood flow to inadequately perfused regions. Quantitative assessment is challenging due to their small size and inter-individual variability not captured by MRI scans. Various models have been created to simulate LMAs [1], differing in interpretation of sparsity and scale of LMAs.

The study aims to depict the probabilistic location of LMAs patient-specifically, understanding collateral flow ramifications. As objectives, we develop a two-part peripheral artery model for explicit LMA placement and optimize LMA configurations using measured flow rate data.

We introduce a peripheral artery model with inlet radii derived from measuring outlets of a reconstructed Circle of Willis model from medical images. The number, location and size of the cortical branch roots are stochastically generated in the proximal portion according to anatomical data [2]. The distal network follows Murray’s law for physiological consistency. The model's structure and peripheral resistances align with medical observations and literature values [3] respectively.

The optimization uses 4D-flow MRI data for proximal blood flow and Single Photon Emission Computed Tomography (SPECT) data for distal perfusion in six vascular territories. Using genetic algorithm, spatial arrangement of LMA becomes the decision variable, while the cost function compares SPECT-derived perfusion rates with computed distal flow rates. Iteratively adjusting LMA location, we alter blood flow redistribution across territories, such that computed flow rates satisfy measured SPECT data in each perfusion region.

Moving forward, the authors aim to compare the optimization effectiveness and computational efficiency of genetic algorithm and binary particle swarm optimization algorithm. The latter method represents each potential LMA connection as a dimension in the particles’ positions within the search space, enabling management of individual LMAs within an arrangement.

The case study involves patients with a stenosed internal carotid artery (ICA). Once the cost function falls below a threshold relative to the SPECT flow rate, indicating recreation of measured blood flow redistribution, the validated arrangement of LMAs is examined. The spatial density, radius, and distribution of LMAs across vascular regions correspond to reported values. The authors plan to further validate the model by comparing it to previous studies, such as models generated using constrained constructive optimization algorithm.

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MODELLING OF 3D WOVEN TEXTILE REINFORCED CEMENT COMPOSITES RVES

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ABSTRACT

Textile reinforced cement composites (TRC) use fibre textiles instead of steel reinforcement. Doing so, thinner and more free-form concrete elements can be produced with higher resource efficiency. While 2D textiles are state of the art, the integration of transversal connections to create 3D textiles improves not only the manufacturing process but also the mechanical bending behaviour of TRC elements. 3D woven textiles have shown relevancy in the construction world due to the cross-sectional optimisation they allow [1]. Models have to incorporate the 3D nature of the reinforcement to properly account for the interactions with the (cracking) cementitious matrix. 3D through thickness models with an explicit representation of the through thickness connections are indeed required for this purpose. Yet, no computational model for this type of material architecture has been proposed until now, partly due to the complexity of the woven reinforcement geometry. This contribution will develop a generation procedure to build the geometry of a mesoscale through thickness Representative Volume Element (RVE) model of a 3D woven reinforced TRC. This computational model will aim to assess the mechanical behaviour of the composite material under bending-type loading, determine the internal stress/strain fields, and analyse the interaction of the reinforcement with the cementitious matrix having degrading mechanical properties. To this end, an iterative geometry generation scheme is developed starting from concepts previously used for polymer-based composites. In particular, a geometrical tensioning procedure is applied to a simplified geometrical configuration of reinforcing yarns. This tensioning procedure is further combined with an interpenetration solving procedure to produce 3D woven textiles geometries [2]. A discretisation finite element meshing procedure is subsequently used to create the RVE. It will be illustrated that this modelling procedure can be the basis of future developments and computational prediction for TRC materials with complex textile geometries. Based on RVE simulations under bending loadings using computational homogenisation procedures, the average (macroscopic) behaviour associated with the matrix degradation and the progressive transfer of stresses to the reinforcing textile will be assessed.

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Modern structure-preserving methods for PDEs
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A STRUCTURE-PRESERVING MATRIX-FREE FINITE ELEMENT METHOD

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ABSTRACT

We present a three-dimensional matrix-free finite element method (MF-FEM) which provides an explicit and arbitrary high order approximation of the smooth solutions of the advection-diffusion partial differential equations both in space and time. The scheme allows for an efficient diagonalization of the mass matrix without any loss of accuracy. This is achieved by coupling the MF-FEM formulation in space with a Deferred Correction (DeC) type method for the discretization in time.

We will first focus on the staggered grid MF-FEM scheme for the Lagrangian hydrodynamics. In Lagrangian formulation, the equations are written in a moving reference frame with respect to velocity and internal energy. We will discuss the structure-preserving properties of our scheme, in particular, local conservation of the total energy by means of simple force correction in the momentum update equation. Next, we will present a high-order MF-FEM scheme for the shallow water equations and show that our scheme is well-balanced with a proper choice of numerical stabilization operators.

The MF-FEM implementation is part of the Fierro computational mechanics code which leverages the immense utility of the MATAR C++ library, providing a seamless integration of the Kokkos Performance Portability EcoSystem with MPI for distributed computing.

Recent advances in computational fracture mechanics and failure analysis
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODEL ASSISTED NON-DESTRUCTIVE EVALUATION OF DEFECTS USING TERAHERTZ TIME DOMAIN ANALYSIS

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ABSTRACT

Current and future detectors for high-energy particle physics like those at Large Hadron Collider (CERN) and EIC at Brookhaven National Lab pose high demands for the structural materials in a high-radiation environment where the accumulated radiation dose leads to defects like voids and cracks due to de-gassing and thermal cycling in the polymeric composite materials. In this work, terahertz time-domain spectroscopy (THz-TDS) is used for strain mapping of a polydimethylsiloxane (PDMS) doped with passive highly dielectrostictive strontium titanate (STO). A polarization polarization-dependent analytical model for the correlation of volumetric strain to the measured change in time of arrival for a THz pulse is developed. The model consists of effects due to changes in the dielectrostrictive properties of the composite due to changes in STO particle density and the change in thickness of the sample upon application of strain due to Poisson's effects. The stress relaxation behavior of the composite is studied to avoid change in strain during the measurement window. The analytical model is validated with results using an open hole tensile and a circular edge notch specimen. The THz strain mapping results are compared with a scale-dependent finite element model (FEM) and surface strain measurement using the digital image correlation (DIC) method. The experimental results show sensitivity to material features like particle clumping and edge effects. THz strain map shows good agreement with FEM and DIC results proving the applicability of this technique for surface and sub-surface strain mapping in polymeric composites.

The experimental results for THz-TDS-based volumetric strain maps agree with the results from DIC surface measurements as well as predictions using finite element models. This forms a robust analytical approach for the development of stress mapping and fracture front mapping in multilayer composites. The model inefficiencies at lower strain levels can be understood and mitigated by having better THz sensors and improving the signal-to-noise ratio.

Continuum biomechanics of active systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ELASTIC-INELASTIC SHELLS WITH GROWTH: AN EULERIAN FORMULATION

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ABSTRACT

This contribution introduces a constrained Cosserat-type shell theory adept at integrating viscoelasticity, inelasticity, remodeling, and growth. The theory is formulated by setting constraints on the director vectors which relate to the position vector. The specific free energy of the system is expressed as a function of various factors including the elastic dilatation, elastic mean curvature, elastic Gaussian curvature, and the elastic distortional deformation invariant.

The elastic dilatation is governed by an evolution equation that involves the symmetric part of the velocity gradient and a mass supply term, which is a function of the elastic dilatation and a scalar field. Similarly, the evolution of the elastic distortional deformation invariant is determined by its relation to the deviatoric part of the unimodular elastic distortional deformation tensor and a symmetric, positive-definite, unimodular tensor.

Furthermore, the evolution equations for the mean and Gaussian curvatures are described, taking into account the time derivatives of these curvatures, material constants, and their homeostatic values. The resultant forces and couples are derived from constitutive equations that are consistent with thermodynamics.

Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NOVEL METHOD TO CALCULATE THE LOAD VS. CRACK EXTENSION CURVE AND THE SIMILARITY OF THE LOAD VS. LOAD-LINE DISPLACEMENT CURVE

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ABSTRACT

The crack growth resistance curve is an important curve in fracture mechanics. In order to obtain the crack growth resistance curve, a typical fracture test must measure the load vs. crack extension (F-Δa) curve. In addition to the basic measurement of the load vs. load-line displacement (F-v_LL) curve, additional devices or complex test operations such as partial unloading are necessary to measure the amount of crack extension. Our research proposes a novel method of calculating the F-Δa curve directly from the F-v_LL curve, in which no additional devices or test operations are required. The proposed method is derived based on the energy balance during crack propagation, which can be easily applicable to these non-standard specimens. Several examples of compact tension (C(T)) and middle crack tension (M(T)) specimens are adopted to verify this method. This method is expected to simplify these available standards for measuring crack length. The similarity of F-v_LL curves and F-Δa curves of specimens that have the same configuration and different geometric parameters is found during the verification calculation of the proposed method. It is found that when specimens are identical except for the initial crack length, the shape of the F-v_LL curves or F-Δa curves are similar, but the positions of the feature points (i.e., the maximum load point) are different. For specimens with the same configuration and different geometric parameters, the crack propagation at the same displacement ratio (or stress ratio) point also has a proportional relationship. The influence of different geometric parameters on the similarity of F-v_LL curves and F-Δa curves is analyzed. The method of mutual transformation between F-v_LL curves or F-Δa curves based on similarity is proposed.

AN EFFICIENT ALGORITHM FOR CALCULATING VIBRATION MODES WITH NON-CLASSICAL DAMPING

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ABSTRACT

With the widespread application of dampers in large structures, how to evaluate vibration modes of large-scale damping systems has become an important issue.
A new computing method for vibration modes of large scale linear non-classical damping systems arising in FEA (Finite element analysis) called quasi-symmetric Lanczos method is proposed. The method can solve complex eigenvalue problems using the quasi-symmetric condition,
The complex quadratic eigenvalue problem (λ^2*M+λ*C+K)u=0 with non-classical damping of order n can be converted into a symmetric eigenvalue problem Av=λ*Bv of order 2n, in which v=[u,λu]^T, A=[-K,0;0,M] and B=[C,M;M,0]. Because matrix A and B are both indefinite matrices, we cannot use conventional method for positive definite matrix to solve it.
The matrix A can be congruently transformed into the J-matrix (J=diag(1 or -1)), while matrix B is still an indefinite symmetric matrix P. We can further convert the eigenvalue problem Jw=λ*Pw into w = λ*inv(J)Pw or w = λ*Dw. The offdiagonals of D=inv(J)P are either symmetric, i.e., d_ij=d_ji, or anti-symmetric, i.e., d_ij=-d_ji. We call D as a quasi-symmetric matrix.
For large scale problems, nonsymmetric Lanczos method is a feasible way to find a few meaningful eigen pairs. It reduces the large-scale eigenvalue problem w = λ*Dw into a small-scale eigenvalue problem w = λ*Tw with T as a tri-diagonal matrix. Conventionally, both left and right Lanczos vectors are computed in nonsymmetric Lanczos method. But when D is a quasi-symmetric matrix, the left Lanczos vectors and right Lanczos vectors also have a quasi-symmetric property. The left Lanczos vectors can be directly assigned via the right Lanczos vectors, so only one side Lanczos vectors are computed. The restarting and the orthogonal operation of the conventional nonsymmetric Lanczos method can also be simplified by the quasi-symmetry.
Finally, we can evaluate the vibration modes of large scale

ACCELERATING STRUCTURAL OPTIMIZATION USING GRADIENT ONLINE LEARNING AND PREDICTION

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ABSTRACT

Unconstrained and constrained optimization problems are typically solved via some form of iterative processes in which all the design variables are updated repetitively. The update of the design variables is usually conducted along one search direction with a step size or length. Thus, it is important to determine the search direction. In the gradient-based optimization method, such search direction can be determined in terms of the gradients of both objective and constraint functions. However, for some problems, computing the gradients of both objective and constraint functions can be computationally expensive or even prohibitive. One such an example could be structural optimization problem, as a subset of constrained optimization, in which the geometry and size and the scale and complexity of physics involved could make the gradient determination computationally expensive or even prohibitive. The challenges may come from material and geometrical nonlinearity, time dependency, multiple scale, or even multiple physics. In this study, we propose a method that can accelerate the optimization process via machine learning, specifically via gradient online learning and prediction (GoLap). GoLap provides a straightforward framework of implementing the online training and online prediction of a one-hidden-layer neural network (NN) into routine iterative optimization process. In GoLap, the online training of the NN is performed in routine iterations using the available historical gradients as training samples; and the online prediction of the trained NN is activated in selected iterations to predict the gradients by running a rapid forward calculation. This method substantially can significantly reduce the overall computational time used to solve a structural optimization problem with fixed step size. Furthermore, GoLap has also been implemented into the algorithms based on the steepest and conjugate gradient descent methods to accelerate optimization process. GoLap has been implemented into the solid isotropic material with penalization method, accelerating the topology optimization for solving 2D and 3D minimum compliance designs problems [1], 2D compliant mechanism design problem with design-dependent load [2], and reliability-based minimum compliance and minimum volume design problems [3].

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Contact and interface mechanics: Modeling and computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MORTAR-BASED ISOGEOMETRIC MODEL FOR PARTIALLY LUBRICATED CONTACTS

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ABSTRACT

Fluidic lubricants are commonly used to reduce friction in tribological systems like bearings and gears. The basic concept is that the lubricant forms a thin film separating the solid surfaces in contact, indirectly transmitting the contact force. Present research primarily focuses on fully lubricated contacts, where lubricants are supplied sufficiently without specific quantity control. However, our research group's experimental results suggest that a significant reduction in the coefficient of friction (COF) can be attained with minimal lubricant application. In such cases, the tribological system is partially lubricated, meaning that the narrow gap between solid bodies is only partially filled with lubricants, whereas air pockets occupy the remaining space. The problem's complexity is further increased when the lubricant cannot withstand the high external load, leading to the coexistence of solid contacts and the fluid film. Modeling this complex contact interface is challenging due to the interaction of multiple mechanisms: the solid deformation, the frictional contact, and the mixture flow of the lubricant and air pockets. In order to address these challenges, this work presents a new model for partially lubricated contacts, integrating the mortar method with NURBS-based isogeometric analysis.

In this model, the Reynolds equation, supplemented by the JFO boundary conditions, is utilized to characterize the multi-phase flow, leading to a complementarity problem with inequality constraints. A cavitation formulation is developed to address this. It employs the Augmented-Lagrangian (AL) method, transforming the complementarity problem into an unconstrained form. Additionally, a frictional contact formulation derived from the AL method is implemented to compute potential solid contacts effectively. The model also accounts for large solid deformations, which could be attributed to asperity contact and high fluid pressure.

A monolithic coupling approach is adopted in this model, allowing for the concurrent solution of all variables from both the fluid and solid components. The resulting formulations are discretized within the NURBS-based IGA (Isogeometric Analysis) framework. Notably, the lubricated contact interface is discretized using the mortar method, facilitating the use of inconsistent NURBS meshes for the solid bodies and the fluid domain. This feature is crucial as the fluid domain often necessitates finer meshes to capture the mixture flow behaviors accurately.

The developed model provides a comprehensive representation of lubricated contact, aiming to enhance the understanding of its fundamental mechanisms and to investigate the impact of the lubricant quantity on the COF.

Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPROXIMATE VORONOI DIAGRAMS FOR NODALLY INTEGRATED GALERKIN MESHFREE METHODS

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ABSTRACT

The application of approximate Voronoi diagrams [1] to nodally integrated Galerkin meshfree methods is presented. Instead of generating exact Voronoi cells as nodal representative domains, the input geometry is pixelated by uniform background cells, and approximate Voronoi cells are obtained by allocating the background cells to the corresponding nodes. As compared to nodal integration using exact Voronoi cells, the computational cost is significantly reduced, while similar accuracy can be achieved. The accuracy is much higher than that of nodal integration using nonconforming cells. This presentation will first briefly review the three categories of domain integration for Galerkin meshfree methods, which include integration by quadrature, integration by stress points, and nodal integration [2]. This presentation will then explain why nodal integration is used for problems with drastic topological changes such as ballistic impacts and natural disasters [2]. The limitations of the current nodal integration techniques will then be presented, which include the impractically high computational cost if exact Voronoi cells are used, and the poor accuracy if nonconforming cells are used. The construction of approximate Voronoi cells will then be presented, which includes the radius expansion algorithm, and a novel way of identifying background cells inside the input geometry. After that, nodal integration using approximate Voronoi cells will be presented, by reusing the integration results, the number of integration performed is very low compared to the number of background cells. After that, several examples are shown to demonstrate the high accuracy and low computational cost of nodal integration using approximate Voronoi diagrams. This research contributes by making nodal integration using Voronoi diagrams computationally practical, and recovers the meshfree nature. The huge sacrifice in accuracy by using nonconforming cells is no longer necessary. Hence this research can lead to increase in computational efficiency for nodally integrated meshfree methods, therefore improve the capability of simulating solid mechanics problems with drastic topological changes.

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Recent advances in high-order methods for computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GENERALISATION OF THE SPECTRAL DIFFERENCE SCHEME FOR THE DIFFUSED-INTERFACE FIVE EQUATION MODEL

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ABSTRACT

High-fidelity simulations of multi-phase flows represent a crucially relevant tool in the design process of many different fields of engineering applications. The sudden change of density, viscosity and thermodynamic properties at the interface between two immiscible fluids poses a great challenge in terms of numerical modelisation. The development of reliable, accurate and robust discretisation techniques to deal with these types of problems consequently represents an unavoidable step to uncap the simulation of challenging scenarios as the ones commonly encountered in the aeronautical industry.

In the present work the spectral difference scheme is employed in the discretisation of the five equation model equipped with the additional Allen-Cahn regularisation terms for interface capturing purposes [1,2]. Within the framework of the spectral difference scheme, in order to mitigate pressure oscillations in proximity of material interfaces in two-phase flows, a change of variables (from conservative to primitive) in the extrapolation to the flux points step is used in order to alleviate the non-linearity of the stiffened-gas equation of state.

A series of numerical test of increasing complexity is considered in order to assess the robustness of the solver, including both kinematic and two-phase test cases. From the former group, the Rider-Kothe vortex is studied in order to quantify convergence properties of the scheme and mass conservation errors. In terms of two-phase flows, a series of more complex problems are considered: the Rayleigh-Taylor instability, a shock-droplet interaction and a three-dimensional, two-phase version of the Taylor-Green Vortex problem.

Overall, the proposed approach showed a good robustness in dealing with a large variety of classical test cases in the two-phase simulation community, advocating the advantages in using high-order discretisations.

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Fluid-structure interaction in interface and moving boundary problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CELL AGGLOMERATION FOR CUT CELLS IN EXTENDED DISCONTINUOUS GALERKIN METHODS

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ABSTRACT

Extended Discontinuous Galerkin (XDG) methods are advanced high-order techniques designed to solve multiphase problems characterized by jumps and kinks at interfaces. In the treatment of these discontinuities, XDG methods embrace a sharp interface approach and implement a cut-cell structure, in which complex geometries are immersed in a Cartesian grid to simplify mesh generation.

However, this approach can result in arbitrarily small cells due to the intersection of background cells with the interface, which cause discretization difficulties because of their diminutive size. In addition, if the size of the immersed geometries changes over time, topological inconsistencies in the mesh structure can occur at different time steps.

To account the issues associated with small-cut cells and topological changes, we present a cell agglomeration approach for XDG methods and tailor it for large-scale simulations. This approach merges problematic cells with suitable neighbors and has been acknowledged as a simple and convenient method [1]. However, it is important to note that cell agglomeration becomes challenging in three-dimensional space due to the high degree of neighborship between cells [2]. In addition, it can create cumbersome problems in large computational simulations, such as the formation of agglomeration chains and ineffective exchange of information in parallel, which are often considered drawbacks in implementations.

In our work, we provide a comprehensive strategy for the typical issues associated with cell agglomeration in three-dimensional and multiprocessor simulations. The proposed strategy is implemented into the open-source software package BoSSS [3] and tested with large-scale simulations of immersed boundary flows.

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Advance and application of meshfree methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CONSTRAINED INTERPOLATION FROM SCATTERED DATA WITH RADIAL BASIS FUNCTIONS

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ABSTRACT

Radial basis functions (RBFs) are a powerful tool for constructing high-order accurate interpolants of scattered data in arbitrary dimension and on manifolds. We present a method of constructing RBF interpolants using constraints to ensure that properties such as, e.g., integral conservation or local bounds, are preserved. We defined a constrained quadratic minimization problem that combines possibly non-linear constraints with RBF interpolation. We demonstrate the method for applications of scattered data interpolation on the sphere.

Current trends in phase-field modeling and computations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING DYNAMIC DUCTILE FRACTURE AND THERMAL SOFTENING WITH A VARIATIONAL PHASE-FIELD FRAMEWORK

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ABSTRACT

A variational phase field model for ductile dynamic fracture is presented. The model is designed for elasto-viscoplastic materials subjected to rapid deformations in which the effects of heat generation and material softening are dominant. The variational framework allows for the consistent inclusion of plastic dissipation in the heat equation, coupled with mechanisms for thermal softening. The model employs a coalescence function that actively degrades fracture energy in conditions characterized by high plastic flow. The plastic yield surface is characterized by a variationally consistent form of the Johnson-Cook model developed for use with the model. A remeshing algorithm is applied to address mesh distortions from the combination of high plastic flow and damage, particularly evident in shear band formation. A distinctive feature of this model is its treatment of damage failure and shear band failure as two separate failure modes, each with distinct indicators for their initiation. The model's efficacy is demonstrated through a series of benchmark problems in dynamic ductile fracture. In particular, the ability of the model to regularize shear band formation and subsequent damage evolution in two and three-dimensional problems is demonstrated. Notably, these phenomena are captured intrinsically through the model's physics, eliminating the need for externally imposed criteria, such as stability thresholds, for the onset of shear band formation.

GRAPHS AND MIXED ADJOINT/DIRECT APPROACHES FOR DESIGN SENSITIVITY ANALYSIS WITH TRANSIENTS AND HISTORY DEPENDENT MATERIAL RESPONSE

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ABSTRACT

The direct (forward) and adjoint (reverse) approaches are popular analytical sensitivity analysis methods which play prominent roles in design optimization and inverse/identification analyses. We present a graph-based mixed adjoint/direct method that enjoys some of the simplicities of the direct method and efficiencies of the adjoint method. It is particularly well suited for systems with transients and history dependent material response due to its straightforward implementation. Indeed, adaptive time-stepping algorithms and various constitutive models are readily accommodated. The computed sensitivities are consistent with the discretize and differentiate approach and as such pass the Taylor verification test. We demonstrate its effectiveness by computing shape and material parameter sensitivities for structures modeled with J_2 plasticity.

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Boundary element methods: New theories and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ELASTIC WAVE DIFFRACTION IN MULTI-DOMAINS WITH A GUNTER-COSTABEL A SYMMETRIC REGULARIZED BOUNDARY ELEMENT METHOD

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ABSTRACT

This work presents a multifaceted contribution to computational elastodynamics in three dimensions. Firstly, it relies on a robust variational formulation of the boundary integral equation tailored specifically for multi-domain scenarios. This formulation marks a significant contribution, enhancing the applicability of elastodynamic simulations using the boundary element method. Secondly, it employs extensive use of surface integration by parts techniques, effectively transforming the computational framework from one reliant on strong and highly singular quadrature to one that adeptly handles weakly singular quadrature. Finally, the study explores the computation of dynamic stress intensity factors, examining their intricate relationship with frequency and stiffness ratio between inclusions and the surrounding matrix.

Advanced numerical techniques for fluid flow in porous media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A PREDICTOR-CORRECTOR SECOND-ORDER TIME-STEPPING SCHEME FOR MODELING WATER FLOW AND SOLUTE TRANSPORT IN UNSATURATED POROUS MEDIA

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ABSTRACT

It is vital to model water flow and solute transport in unsaturated soils to comprehend and manage different environmental phenomena. The Richards equation is used to model water flow and is combined with the equilibrium advection-dispersion equation for solute transport. Several second-order time-stepping schemes have been developed for solving the coupled system (Kamil et al., 2024; Toutlini et al., 2024). The objective of this study is to numerically solve the coupled model by utilizing special temporal schemes in conjunction with standard and non-standard Galerkin finite element methods for spatial discretization. At each time level, we address the Leverett equation to derive the initial estimate of the pressure head. Subsequently, employing this initial estimate, we solve the Richards equation to obtain a more refined second approximation of the pressure head. The final prediction of the pressure head is corrected using these two approximations. The solute transport equation is then solved with the water content and flux that are derived from the Richards equation solution. The proposed schemes differ in their treatment of the Leverett equation. In a first approach, a constant pressure head is assumed within each element. However, to overcome discontinuities associated with this method, a smoothness technique has been adopted. This involves projecting the discontinuous pressure head onto the space of linear piecewise polynomials, resulting in a continuous profile. In contrast, a second approach considers a linear pressure head within each element, offering an alternative method to handle the Leverett equation. The proposed schemes offer distinct advantages due to the linear nature of the resulting system, facilitating easy implementation, parallelization, and avoiding the issues associated with the divergence of iterative schemes. We assessed the effectiveness and robustness of our approach through a series of numerical experiments. The results provide compelling evidence that confirms the efficiency of the proposed methods. In general, the second method shows better stability and accuracy for both homogeneous and heterogeneous soils. This implies that, in comparison to the first method, taking into account a linear pressure head within each element produces more consistent results, particularly when handling different soil properties.

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Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THIN WAVEGUIDES WITH ROBIN BOUNDARY CONDITIONS

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ABSTRACT

We consider the Laplace operator in a thin three dimensional tube with a Robin type condition on its boundary and study, asymptotically, the spectrum of such operator as the diameter of the tube's cross section becomes infinitesimal. In contrast with the Dirichlet condition case, we evidence different behaviors depending on a symmetry criterium for the fundamental mode in the cross section. If that symmetry condition fails, then we prove the localization of lower energy levels in the vicinity of the minimum point of a suitable function on the tube's axis depending on the curvature and the rotation angle. In the symmetric case, the behavior of lower energy modes is shown to be ruled by a one dimensional Sturm-Liouville problem involving an effective potential given in explicit form.

Model order reduction for parametrized continuum mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

WLASDI: WEAK-FORM LATENT SPACE DYNAMICS IDENTIFICATION

April Tran[1], Xiaolong He[2], Daniel Messenger[1], Youngsoo Choi[3] and David Bortz[1]*

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ABSTRACT

Reduced order modeling is inspired by the need to address the computational and mathematical challenges posed by simulating complex, high-dimensional systems in various scientific and engineering domains. To address this, we introduce WLaSDI: Weak-form Latent Space Dynamics Identification, a data-driven projection-based reduced order model (pROM) simulation method that incorporates weak-form equation learning algorithms. Extended from LaSDI: Latent Space Dynamics Identification, WLaSDI first compresses data, then projects onto the test functions and learns the local latent space models. With WLaSDI, the local latent space is obtained using weak-form equation learning techniques. Notably, WLaSDI demonstrates significantly enhanced robustness to noise. Compared to the standard sparse identification of nonlinear dynamics (SINDy) used in LaSDI, the variance reduction of the weak form guarantees a robust and precise latent space recovery, hence allowing for a fast, robust, and accurate simulation. We demonstrate the efficacy of WLaSDI vs. LaSDI on several common benchmark examples including viscid and inviscid Burgers', radial advection, and heat conduction.

Geometric mechanics formulations and structure-preserving discretizations for continuum mechanics and kinetic models
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GEOMETRIC FORMULATION OF THREE-TEMPERATURE RADIATION HYDRODYNAMICS

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ABSTRACT

Radiation hydrodynamics is the study of the hydrodynamics of a fluid interacting with a radiation field, finding application in fields such as astrophysical hydrodynamics and inertial confinement fusion. The governing equations for three-temperature (3T) radiation hydrodynamics consist of fluid equations for an electron-ion fluid coupled to a radiation field, forming a complicated set of PDEs containing advection, diffusion, and strong nonlinear interaction terms. As such, the discretization of this system is a challenging problem and an active area of research. With the aim of developing geometric structure-preserving integrators for the simulation and optimal control of the 3T system, we develop a geometric formulation of 3T radiation hydrodynamics using a port-Hamiltonian framework. This gives a geometric framework for understanding the conservative properties of the 3T system. We further show that the 3T system is an irreversible port-Hamiltonian system, where irreversible internal entropy production arises from fluid-radiation interaction and diffusion. Finally, we develop a metriplectic formulation of the flux and the interaction terms.

Performance-portable algorithms for unstructured mesh applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FOUR-DIMENSIONAL PARALLELIZATION ENHANCED WITH ADAPTIVITY AND BATCHING FOR THE SOLUTION OF PHONON BOLTZMANN TRANSPORT EQUATION

Han Tran[*1], Siddharth Saurav[2], Sandip Mazumder[2], P. Sadayappan[1] and Hari Sundar[1]*

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ABSTRACT

The phonon Boltzmann transport equation (BTE) is suitable for modeling heat transport at submicron scales in semiconductor materials. However, the BTE is a seven-dimensional equation, bringing in challenges in parallelization regarding load imbalance due to the linear systems' conditioning variation. Furthermore, applications of the BTE solution, e.g., simulation of frequency-domain thermo-reflectance (FDTR) experiments, often require thousands of time-steps to obtain meaningful physical quantities, resulting in long time-to-solution. Here, we first present the combined band+cell-based method, which combines parallelization in frequency and spatial dimensions for the BTE solution [1]. The advantages of this approach are the inconsiderable communication costs (only reduction is required) in the frequency parallelization and the high level of parallelism in the spatial domain. Next, we present the batching technique that groups multiple linear systems into a batched system solved simultaneously. This technique merges many small MPI messages into a larger one, reducing communication overhead when the grain size of spatial parallelization becomes small. We also discuss our recently developed adaptive algorithms to minimize the load imbalance in frequency parallelization and the unnecessary computations in the batching technique of spatial parallelization. Finally, we present the numerical experiments simulating heat transports in semiconductor devices via the BTE solution, demonstrating that our developed methods achieved excellent speedups and maintained scalability up to 25k cores.

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Mathematics and algorithms for predictive digital twins (DT)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MACHINE LEARNING FRAMEWORK FOR MODEL CALIBRATION OF MERCURY TARGET SIMULATION

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ABSTRACT

As the most powerful pulsed spallation source in the world, the Spallation Neutron Source (SNS) at the Oak Ridge National Laboratory (ORNL) uses liquid elemental mercury as the target material to generate neutron beam lines for scientific and engineering discoveries. Due to the severe working condition, the mercury targets were prone to leak prematurely causing several interruptions to the SNS user program. The mercury constitutive model predicting the strain and stress in the target vessel plays a central role in improving the lifetime prediction and future designs of the targets at the SNS. In this effort, we leverage the experiment strain data collected over multiple years to improve the mercury constitutive model through a combination of large-scale simulations of the target behavior and the use of machine learning tools for surrogate modeling. We present two interdisciplinary approaches for surrogate-based calibration of expensive simulations using evolutionary neural networks and sparse polynomial expansions. The newly calibrated simulations achieve remarkable improvement on the prediction accuracy compared to previously reported reference parameters and can aid in fatigue analysis for more accurate estimation of the mercury target lifetime.

Advanced materials: Computational analysis of properties and performance
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL STUDIES OF COMPRESSION FAILURE IN TRIPLY PERIODIC MINIMAL SURFACE-BASED CERAMIC FOAMS

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ABSTRACT

Microstructures with minimal surfaces can be often found in natural porous architectures, where the surface tension minimizes the area. The triply periodic minimal surfaces (TPMS) [1] are an example of such microstructures with minimal surfaces. Compared with other porous structures, TPMS have three significant features: firstly, their geometries can be completely expressed via analytical functions; secondly, TPMS are periodic in three independent directions and thirdly, the mean curvature of TPMS is zero [2]. Transforming the TPMS-based unit cell into a lattice structure has particular usage in aerospace, nuclear energy, and biomedical applications where light weight, high stiffness, and temperature resistance are of critical importance. In the presented studies, the linear elastic and failure behavior of four typical TPMS structures (Primitive, Gyroid, Neovius, and IWP) under compression were studied using finite element analysis. Numerical modeling of the damage propagation and strength prediction was provided by removing the finite elements in which the appropriate damage criterion is reached. Utilizing the equations of the generated TPMS structures, the wall thickness of unit cell was considered the main parameter that defined the ceramics volume fraction and should be taken into consideration. Therefore, various unit cell models for different wall thicknesses were generated and used to investigate the impact of the cell geometry on the damage initiation, propagation, and the overall compression strength. The results of compression strength and damage development were compared with those of other TPMS structures for the same wall thickness and volume fraction. Finally, the periodic repetition of TPMS unit cells was used to evaluate and understand the effect of boundary conditions on damage evolution on the macroscale.

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Verification techniques in computational physics and applied mathematics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DETERMINISTIC VERIFICATION OF ELECTROSTATIC, GYROKINETIC PARTICLE-IN-CELL CODES USING THE METHOD OF MANUFACTURED SOLUTIONS

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ABSTRACT

As the scope and complexity of particle-in-cell (PIC) algorithms in plasma simulation continue to grow, the need for a robust and straightforward method to verify the correctness of PIC implementations becomes crucial. This presentation introduces a deterministic approach for rigorously verifying multidimensional, electrostatic, gyrokinetic particle-in-cell codes, utilizing the method of manufactured solutions. Our method demonstrates that thorough verification can be achieved by exclusively scrutinizing errors in grid quantities, enabling a lightweight and non-intrusive integration into existing particle-in-cell codes. The validity of our theoretical assertions is confirmed through numerical results obtained in XGC.

A FEASIBLE NUMERICAL MODEL FOR AN ANALYSIS OF A PIPE-LAY ON A ROUGH SEAFLOOR

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ABSTRACT

Submarine pipelines for the transportation of hydrocarbon fluids may spread hundreds to thousands of kilometers and are usually installed by lowering them down from the laying vessel. During this process, the pipelines are subjected to different types of loading, which should be given proper consideration in the pipeline design.
By default, a common practice to analyze pipelines in their installation is by considering a horizontal flat seafloor. In reality, however, the bathymetric maps of the sea bottom reveal faults, folds, and on-bottom channel systems. Those seafloor irregularities and potential pipeline crossings may result in severe stress concentrations within the pipelines, eventually leading to pipeline failure.
Analyzing a pipe-lay on a rough seafloor, however, is much more computationally involved since the pipe-lay front configuration, as well as its internal forces, are continuously changing throughout the pipe-lay process, such that considering solely a typical steady-state configuration at the pipe-lay front is no longer sufficient. To ensure pipeline integrity during the installation, it is essential to obtain internal force envelope diagrams, which provide the historical maximum and minimum force bounds at every location along the pipeline throughout the entire pipe-lay proceeding.
This work presents a feasible, simple numerical technique compliant with the adaptation of any possible load induced by the environment for calculating the internal force envelope diagrams. The entire pipeline is modeled as a single continuous segment considering geometrical nonlinearity induced by large deformations. Following the actual pipe-lay process, the numerical solution is proceeded sequentially by an incremental increase of the pipeline length and consistent minimization of the total potential energy of the system discretized as a Riemann sum, solving the subsequent algebraic system of nonlinear finite difference equations by a Newton-Raphson technique [1-2]. The feasibility of the proposed technique is demonstrated through several scenarios of a pipe-lay across the basic types of seafloor irregularity [3].
The proposed technique presents an efficient, time-saving alternative to the available general- and special-purpose commercial software, allowing the user, by developing his own in-house code, to take full control over the calculations.

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WEAK-FORM GAUSSIAN PROCESS-BASED LATENT SPACE DYNAMICS IDENTIFICATION

Margaret Trautner[*1], Xiaolong He[2], April Tran[3], Youngsoo Choi[4] and David Bortz[3]*

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ABSTRACT

Recent work in model order reduction has introduced an algorithm called LaSDI (Latent Space Dynamics Identification) as a tool to accelerate physical simulation by learning latent space dynamics. In many problems, high dimensional time series data may be driven largely by the dynamics of a latent space with lower dimension, and the LaSDI algorithm takes advantage of this dimension reduction. The original LaSDI algorithm uses SINDy (Sparse Identification of Nonlinear Dynamics) as a subroutine for symbolic latent space dynamics identification. However, symbolic learning is not robust to the presence of noise in the data; in response, additional work proposed WLaSDI, (Weak-Form LaSDI) which poses the latent space dynamics in weak form, which is shown to be more robust to noise. An additional challenge in dynamics modeling is incorporating parameter dependence. In LaSDI, a solution is linearly interpolated for new parameters between separately learning dynamics for multiple parameterizations. However, separate learning can be expensive, and it is desirable to have uncertainty quantification to inform future sampling. Along these lines, GPLaSDI (Gaussian Process-based LaSDI) uses Gaussian processes to interpolate between various parameters and obtain uncertainty quantification as well. In our work, we combine these two improvements to the LaSDI framework: the weak formulation of the latent space and interpolation with Gaussian processes. Theory is presented and experiments on benchmark problems such as the Vlasov equation for plasma physics are discussed.

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New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION OF VISCOELASTIC LOCAL RESONATORS FOR SANDWICH METASTRUCTURES

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ABSTRACT

Metastructures have gained attention in recent years due to their noise and vibration control properties in tunable frequency ranges, basing their behaviour on the principle of phononic crystals, which exhibit frequency ranges known as bandgaps, in which elastic and acoustic waves do not propagate. Metastructures may be achieved through the inclusion of local resonator elements, which act as vibration absorbers and may be periodically distributed in host structures. The advantage of metastructures using local resonators is that, unlike phononic crystals, the bandgaps are generated based on the properties of the resonator elements. This paves the way towards compact and lightweight vibroacoustic solutions for the lower frequency ranges, since wave propagation and vibratory response can be affected by local resonators of sizes smaller than the host structure's wavelengths. An interesting approach in the investigation of metastructures design is the search for optimal geometries and damping properties for the local resonators, so that they can provide vibration attenuation in wider frequency ranges and/or for relatively distant resonance peaks. That is why this research work proposes a topology optimization strategy to find optimal geometry and damping properties for viscoelastic local resonators, as a building block for application in vibration control of sandwich metastructures. For that, standard topology optimization techniques, such as the Bi-directional Evolutionary Structural Optimization method, need to be adapted in order to simultaneously account for several design criteria, such as static and dynamic structural integrity, resonance frequency tuning and added structural damping. In this work, first, an assessment on different strategies to define a proper objective function for the topology optimization problem is presented. Based on preliminary results obtained so far, non-standard strategies must be considered to obtain well-performing solutions. Then, a discussion on the challenges posed to the methodologies by the viscoelastic behavior of the resonators is put forward. Indeed, the frequency and temperature dependence of viscoelastic resonators properties requires customized optimization techniques for resonance frequency tuning and added structural damping evaluation. Finally, an analysis of the applicability and expected performance of the solutions found for the local resonators when inserted into sandwich metastructures is performed. Given the current interest in the development of metastructures with local resonators making use of additive manufacturing with polymeric materials, which present viscoelastic behavior, it is expected that this work could bring some important contributions to this research area.

Constitutive modeling of complex materials with machine learning and artificial intelligence
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICS INFORMED NEURAL NETWORKS FOR PREDICTING SOFT SOLID DEFORMATION

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ABSTRACT

Mild traumatic brain injury (mTBI) is a silent epidemic and is a major cause of disability and morbidity. Event like mechanical falls, military deployment, contact sports like American football, Rugby, etc., could lead to mTBI. However, still the primary injury-biomechanics remains unclear, novel mechanisms like shear shock formation in brain could provide some clarity [1]. Moreover, the existing finite element based computational solvers are mostly confined to research studies and are not deployable to predict the brain deformation given their computational cost. A real-time estimate of brain deformation in the event of an head impact can provide a quantitative insight towards development of mTBI injury metrics.

With this motivation, the current study aims to develop physics informed fully connected dense neural networks (PINNs) to predict the deformation of an hyperelastic soft solid without using any labelled data. The proposed data-free PINNs model employs an innovative incremental-training algorithm that captures the causality of the physical phenomenon, homogeneous deformation and incompressibility. Utilising non-dimensionalised governing equations to minimise residuals and enforcing the boundary conditions, our approach ensures efficient training of the model. We employ an adaptive training algorithm to incrementally train the model, ensuring satisfaction of governing equations and boundary conditions. The developed PINNs model accurately captures three-dimensional hyperelasticity, focusing on high order hyperelastic models for different homogeneous deformations. Once trained, the model swiftly responds to any spatial coordinate within the physical domain for the specified homogeneous deformation. Three different strain energy density functions were considered: 1) Neo-Hookean, 2) Moony-Rivlin, and 3) Landau (a fourth order elastic model [1]). The data-free PINNs solution for Landau hyperelastic model was compared to the analytical solution, revealing RMSE of 0.04%, 0.08%, 0.16%, 0.18%, 0.07%, and 0.10% for uniaxial tension, uniaxial compression, biaxial tension, biaixal compression, pure shear, and simple shear, respectively. These results affirm the effectiveness of the proposed approach across different deformation cases for Landau hyperelastic model. The success encourages the natural extension of PINNs to capture viscoelasticity in soft solids.

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Advances in damage & fracture modeling of multiphysics materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTATION INFRASTRUCTURE FOR MODELING DISCONTINUITIES WITHIN MATERIALS: DEIP, BEAVER AND MOOSE

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ABSTRACT

This presentation provides an overview of several open-source codes developed within our group for modeling interfaces (such as cohesive zone and Discontinuous Galerkin) within materials. The popularity of discontinuous formulations for computational solid mechanics has steadily increased for physical applications such as fracture mechanics. A common approach for numerically realizing these methods is using the so-called zero-thickness interface finite elements. Unfortunately, standard commercial finite element codes do not contain mesh generation features for zero-thickness elements. Also, the modeling and simulation of complex engineering materials using the representative volume elements (RVE) has become quite extensive, for which periodic finite element meshes are important. However, few mesh generators today will produce such interface elements along the boundary of the periodic RVE, which are needed for modeling behavior such as sliding along grain boundaries in polycrystalline metals. To tackle these challenges, our group has been continually enhancing the Discontinuous Element Insertion Program (DEIP), a MATLAB code for inserting interface elements into two and three-dimensional meshes of all standard element types. Its algorithm is topologically based and requires only nodal coordinates and element connectivity as input. API are provided for meshes from Abaqus, Gmsh, and Cubit formats. Additionally, for modeling the physics of these interfaces, our group has recently developed an application for the MOOSE object-oriented finite element framework, called BEAVER. This application includes realizations of the Variational Multiscale Discontinuous Galerkin (VMDG) method, which provides closed-form expressions of the stability parameters needed for methods such as the interior penalty DG and Nitsche methods. Representative simulations from these codes are provided to highlight various applications.

A TIME-RELAXATION REDUCED ORDER MODEL FOR THE TURBULENT CHANNEL FLOW

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ABSTRACT

Regularized reduced order models (Reg-ROMs) are stabilization strategies that leverage spatial filtering to alleviate the spurious numerical oscillations generally displayed by the classical Galerkin ROM (G-ROM) in under-resolved numerical simulations of turbulent flows. In this paper, we propose a new Reg-ROM, the time-relaxation ROM (TR-ROM), which filters the marginally resolved scales. We compare the new TR-ROM with the two other Reg-ROMs in current use, i.e., the Leray ROM (L-ROM) and the evolve-filter-relax ROM (EFR-ROM), in the numerical simulation of the turbulent channel flow at $Re_{\tau} = 180$ and $Re_{\tau} = 395$ in both the reproduction and the predictive regimes. For each Reg-ROM, we investigate two different filters:

(i) the differential filter (DF), and

(ii) a new higher-order algebraic filter (HOAF).

In our numerical investigation, we monitor the Reg-ROM performance with respect to the ROM dimension, N, and the filter order. We also perform sensitivity studies of the three Reg-ROMs with respect to the time interval, relaxation parameter, and filter radius. The numerical results yield the following conclusions:

(i) In terms of the Reynolds normal and shear stresses, all three Reg-ROMs are significantly more accurate than the G-ROM.

(ii) In addition, all three Reg-ROMs are more accurate than the ROM projection, which represents the best theoretical approximation of the training data in the given ROM space.

(iii) With the optimal parameter values, the new TR-ROM yields more accurate results than the L-ROM and the EFR-ROM in all tests.

(iv) For most N values, DF yields the most accurate results for all three Reg-ROMs.

(v) The optimal parameters trained in the reproduction regime are also optimal for the predictive regime for most N values, demonstrating the Reg-ROM predictive capabilities.

(vi) All three Reg-ROMs are sensitive to the filter radius and the filter order, and the EFR-ROM and the TR-ROM are sensitive to the relaxation parameter.

(vii) The optimal range for the filter radius and the effect of relaxation parameter are similar for the two $\rm Re_\tau$ values.

Predictive digital twins
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HYBRID ANALYSIS AND MODELING FOR TURBULENT FLOW PROBLEMS

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ABSTRACT

The prospect of predictive Digital Twins opens up a lot of application possibilities, but it also brings forth the requirement for efficient and reliable simulators. While reduced order models (ROMs) have been shown to offer excellent speed-up for the approximation of complex physical problems, issues that characterize conventional methods remain true. Constructing ROMs for large problems and/or problems with significant parameterization is often infeasible. Moreover, the power of the reduced model is measured, often inadequately, in terms of how close it can get to the underlying high-fidelity model. In an effort to address such issues, this work will use the hybrid analysis and modeling [1] (HAM) strategy combining multiple reduced order modeling (ROM) techniques and data-driven corrections.

This work will initially consider the construction of a typical hybrid ROM scheme [2], combining the proper orthogonal decomposition (POD) with Galerkin projection and interpolation schemes. Aiming towards as sparse a training set and reduced bases as possible, we use HAM, and more specifically the corrective source term approach (CoSTA). We introduce an extra correction step in the typical ROM online problem that uses a meta-model to evaluate the residual error of the ROM approximation, modify the algebraic problem and improve the final solution.

Finally, the ability of the proposed strategy is measured in terms of computational acceleration and increase in accuracy when approximating turbulent flow around known wing geometries.

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Scientific deep learning
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SELF-SUPERVISED LEARNING FOR HEALTH ASSESSMENT OF LITHIUM-ION BATTERIES IN ELECTRIC VEHICLES

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ABSTRACT

Health evaluation for lithium-ion batteries (LIBs) typically relies on constant charging/discharging protocols, often neglecting scenarios involving dynamic current profiles prevalent in electric vehicles. Conventional health indicators for LIBs also depend on the uniformity of measured data, restricting their adaptability to non-uniform conditions. In this study, a novel training strategy for estimating LIB health based on the paradigm of self-supervised learning is proposed. A multiresolution analysis technique, empirical wavelet transform [1], is utilized to decompose non-stationary voltage signals in the frequency domain. This allows the removal of ineffective components for the health evaluation model. The transformer neural network serves as the model backbone, and a loss function is designed to describe the capacity degradation behavior with the assumption that the degradation in LIBs across most operating conditions is inevitable and irreversible.

The results show that the model can learn the aging characteristics by analyzing sequences of voltage and current profiles obtained at various time intervals from the same LIB cell. The proposed method is successfully applied to the Stanford University LIB aging dataset [2], derived from electric vehicle real-driving profiles. Notably, this approach achieves an average correlation coefficient of 0.9 between the evaluated health index and the degradation of actual capacity, demonstrating its efficacy in capturing LIB health degradation. This research highlights the feasibility of training deep neural networks using unlabeled LIB data, offering cost-efficient means and unleashing the potential of the measured information.

Keywords: lithium-ion batteries, electric vehicles, empirical wavelet transform, transformer, self-supervised learning.

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Recent advances in computational fracture mechanics and failure analysis
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FINITE STRAIN ELASTIC-PLASTIC CRACK ANALYSIS BY USING S-VERSION ISOGEOMETRIC ANALYSIS

Yuhi Tsuchiyama[1], Yusuke Sunaoka[1], Takashi Kurosawa[1], Yuto Otoguro[1] and Hiroshi Okada[1]*

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ABSTRACT

In the presentation, the formulation and the numerical implementation of the s-IGA (S-version Isogeometric Analysis, see [1] for IGA) for finite strain elastic-plastic analysis including elastic-plastic fracture mechanics problem are presented. S-IGA follows the idea of s-FEM (s-version finite element method [2]). IGA patches for the structure/solid as whole and for local features such as cracks are generated separately. They are superposed each other. Such process of building analysis model makes adding local features, such as cracks, to the analysis model very tractable. In a similar way of the thoughts, X-IGA is found to be a popular methodology. S-IGA may be one of alternatives to the existing methodologies.

In the presentation, S-IGA for finite strain elastic-plastic problems is presented. In the present research, a finite strain elastic-plastic constitutive law assuming the multiplicative decomposition of plastic and elastic deformations (see de Souza Neto et al. [3]) is adopted. The hyperelasticity is assumed for the elastic deformation part. In the presentation, the basic equation formulation of S-IGA for finite strain elastic-plastic analysis, its numerical implementation including ways to store the strain history parameters, ways to effectively model the crack, etc., are described. Then, a few example problems and some concluding remarks at present moment will be presented.

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Computational particle-based solvers for multiphysics & multiscale simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE HYBRID RESOLVED-UNRESOLVED SPH(2)-DEM COUPLING SIMULATION FOR THE INTERNAL SOIL-EROSION IN SOIL-STRUCTURES

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ABSTRACT

Internal erosion induced by seepage flow inside the soil accelerates soil failure during a flood disaster. Numerical simulation, which enables microscopic observation through hypothetical numerical experiments, can be an effective tool to quantitatively evaluate the relationship between internal erosion and the instability of the soil-structure.
Fluid-Soil multiphase flow simulation requires coupling technologies that can represent the interaction between soil-particles and fluid and the movement of particles. There are two main concepts for coupling models: "Resolved coupling model," which can calculate detailed flow and fluid forces, and "Unresolved coupling model," which is based on empirical drag and seepage flow models. However, previous studies have indicated that both models should be judged appropriately based on the ratio of solid particle to fluid spatial resolution [1]. However, applying a resolved coupling model to the vast number of soil particles composed of ground is impractical from a computational cost perspective, and empirical unresolved coupling model has difficulty in representing localized failures such as internal erosion [2]. Moreover, to solve the seepage flow accurately using particle methods, it is essential to employ high-order schemes that distribute the particles in an ideal configuration consistent with the space-time varying porosity distribution. Novel coupling models that satisfy both computational accuracy and efficiency are desirable. In this study, we developed a fluid-soil particle coupled model that directly represents the transport of soil particles during the erosion process. That is, it couples a DEM-based soil-particle model with a seepage flow simulation, enhanced by SPH(2) [3]. The proposed method is a hybrid coupled model that suitably employs both resolved and unresolved models depending on the resolution of the soil particles. This paper reports on the verification of the accuracy of the seepage flow simulation with SPH(2) and numerical experiments on internal erosion using the proposed hybrid coupled model.

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Advanced computational modelling of wood, wood-based products, bio-composites, and timber structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DETERMINATION OF ORTHOTROPIC ELASTIC MODULUS OF WOOD BY INDENTATION WITH NONE-AXISYMMETRIC INDENTER AND FEM SIMULATION

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ABSTRACT

Woods are biomaterial and have complex structures. The annual rings are made by seasons. Then, the rigidity of wood is difference along direction. Thus, the elastic modulus of the wood can be considered as the orthotropic material in the macro scale. It is necessary to clarify these mechanical properties in order to expand the range of applications of woods [1]. On the other hand, the indentation method is a quasi-nondestructive testing method and there are many applications to measure the rigidity of materials. In order to give the orthotropic mechanical properties by using an axisymmetric indenter, the indentation test should be made from the different directions. On the other hand, different load-depth data can be obtained by rotating a none-axisymmetric indenter along to an axis normal to a wood surface.

Therefore, in this study indentation tests are performed to woods by using cylindrical indenter with both sides are sphere, that is none-axisymmetric indenter. This indenter is made from aluminum with about 20 mm length and 5 mm radius by using 3D processing machine. Many load-depth curves can be given by rotating the indenter along the normal axis to the wood surface. In order to determine orthotropic mechanical properties, FEM simulations are performed with the parameters as orthotropic elastic modulus along tangential, radial and longitudinal direction of the wood. By minimizing the error between measured and simulated load-depth curves, the orthotropic elastic modululi can be given. The determined orthotropic elastic moduli are compared to the measured ones by using compress tests.

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Multiphase flow and non-Newtonian fluid - Modelling and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL ANALYSIS OF DROPLET FREEZING ON COLD SURFACES USING THE MOVING PARTICLE SIMULATION METHOD

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ABSTRACT

Icing is hazardous to in-flight aircrafts because the ice disturbs airflow around the airfoil, decreases the aerodynamic performance, and in some cases, forces the aircraft to be uncontrollable. Established numerical tools for icing prediction are based on Euler grid methods. They can predict rough estimates of ice thickness over a large surface, for example a whole wing, at low cost. However, icing in some conditions, for example, when supercooled large droplets (SLD) splash on the aircraft surface, or when complex shaped ice is formed, are difficult to predict. The reason is because some key mechanisms of ice formation, namely droplet merging, accumulation, and freezing, are not fully described. The moving particle simulation (MPS) method is effective in solving free surface flow. Droplet dynamics involving splitting and merging can be simulated with no special treatment. We therefore expect that the MPS method is a potential means to improve the physical fidelity of icing prediction.

In this presentation, extensions to the explicit-MPS method for solving freezing problems, and validations through analyses of droplet freezing, will be described. To solve the thermodynamics of a freezing liquid, we adopted a common approach that is used in the nuclear engineering field (e.g. Koshizuka et al, Int Conf Nucl Eng, 2001). Surface tension and wettability was introduced by our original surface-tension-as-pressure model (Tsujimura et al., Comput Particle Mech, 2023). As the first validation of our MPS code, a one-dimensional heat conduction problem and a freezing front propagation problem was solved, and the time-dependent results agreed well with theoretical solutions. Second, a sessile droplet freezing on a cold plate was solved. Theoretically, the frozen droplet’s shape becomes either concave up or concave down depending on the surface wettability and the liquid-solid density ratio. The ices’ shapes were successfully predicted. As the third validation, a droplet impinging on a flat surface was simulated. The droplet bounded in a room temperature condition while it adhered to the plate in a supercooled condition, which are behaviors that agree with an experiment (Zhang et al., Int J Heat Mass Transfer, 2020). The droplet’s overall shape during impact was qualitatively similar to the experiment. The presentation will demonstrate our initial attempt of applying the MPS method to icing problems.

Deep and machine learning methodology in the context of application to computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREDICTION OF UNSTEADY HEAT TRANSFER OF TEMPERATURE FIELD ON A CIRCUIT BOARD USING SUB-VOXELS INPUT DATA STRUCTURE

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ABSTRACT

In recent years, CAE analysis has reduced the number of experiments and costs in the design process of manufacturing. However, CAE analysis for high accuracy is computationally expensive. The prediction by machine learning would be expected to be accurate as same as CAE and shorter time than CAE. In general, it is difficult to predict extrapolation in regression problems. Rules-based on physical phenomena should be well-trained in the predictor for extrapolation. Therefore the predictor is required to improve generalization performance and adapt to engineering problems.

In our previous study, we proposed a method for constructing a surrogate model to analyze the temperature distribution on a circuit board with ICs. The input data consists of the positional relationship between different ICs placed on the board and the coordinate values of the evaluation points and ICs. In this study, the predictor computes a temperature at a point using local differential physical quantities and local material properties. We'd like to propose a new training technique using the sub-voxels which is a container of local physical quantities and material properties as input parameters in the analysis field. The predictor can extrapolate the physical temperature field because physical rules are trained in the predictor. The objective of this study is the construction of a surrogate model that continuously predicts an unsteady temperature field on a circuit board using sub-voxels input data structure.

The input matrix which is configured using sub-voxels is suitable for convolutional neural networks. The predictor was composed of a CNN. The advantage of the sub-voxels is that a large amount of training data can be obtained from a single analysis result. Dummy temperatures for ICs were created to extract initial temperature features. The low-temperature data was down-sampled to eliminate bias in the data distribution. Thus, the accuracy of the predictor was improved and the training cost was reduced. We will discuss effective input data design to improve prediction accuracy and reduction of training computation.

Multiscale methods for advanced manufactured materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREDICTION OF THE EFFECTIVE RESPONSE OF CARBON-BLACK/ULTRA-HIGH-MOLECULAR-WEIGHT-POLYETHYLENE NANOCOMPOSITES BY MULTISCALE NUMERICAL MODELS

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ABSTRACT

Stanislav Buklovskyi, Kateryna Miroshnichenko, Igor Tsukrov (University of New Hampshire, USA)
Rebecca Thomson, Peder Solberg, Douglas Van Citters (Dartmouth College, USA)

The incorporation of carbon nanoparticles into ultra-high-molecular-weight-polyethylene (UHMWPE) provides opportunities for multifunctionality, such as increased electrical and thermal conductivity, as well as potential improvements in mechanical properties, including stiffness and wear resistance. In this study, we developed mesoscale numerical models of carbon-black (CB) reinforced UHMWPE based on micro-computed tomography (μCT) images of the material. The models incorporate the CB-containing layers around UHMWPE granules observed in the μCT images. These layers are treated as two-phase composites, and their properties are evaluated using analytical micromechanical schemes.

Mesoscale models of representative volume elements are analyzed by the finite element method. Numerical predictions of the overall elastic and thermal properties of the composites are compared with experimental measurements conducted on the same material systems, consisting of UHMWPE with various weight fractions of CB, ranging from 0.5% to 10%. The results emphasize the importance of incorporating accurate information on the distribution of carbon particles in the composite for the precision of the numerical models.

Acknowledgments

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Mechanobiology of cells, vesicles and biomembranes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING OF CELL CORTICAL TENSION BY A CO-DYNAMICS MODEL OF ACTIN, MYOSIN AND CROSSLINKER IN ACTOMYOSIN CORTEX

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ABSTRACT

The cell membrane comprises plasma membrane and actomyosin cortex with their linker proteins. The actomyosin cortex, a composite material of actin filaments, myosin mini-filaments and crosslinkers, plays an important role in regulating a membrane stiffness. The myosin moves over actin filament through molecular interactions between the myosin head and actin, and this local event generates local contraction of cortex that results in cortical tension. A regulation of cortical tension is a crucial issue for various cell motions, and a recent study has shown its spatial difference also contributes the regulation [1]. However, how each of filaments mechanically works during generation of cortical tension remains unclear. Some mathematical models have been proposed to tackle this question (e.g., [2]); however, a comprehensive model being across different scales from filament to cell level has not been developed. In this study, we propose a mechanical model of a cellular-scale actomyosin cortex composed of multiple filaments. Line elements including resistances in stretching and bending are applied for dynamics of actin filaments, where their interconnection via crosslinkers is modeled by a spring element. The myosin mini-filament is modeled by a spring element that interconnects with actin filaments, and its sliding motion over the actin filament is described as a relative motion of myosin head to the actin filament. To reproduce a realistic structure and tension in cell cortex, the filaments are initially distributed within a domain of thin spherical shell, and a simulation is carried out until quasi equilibrium is reached. Present results showed overall cortical tensions increase as the number of myosin filaments and crosslinkers increase that is consistent with an experimental trend [3], and deformation of actin filaments has relatively little effect on generation of the cortical tension than those of myosin and crosslinkers. Our results also suggest that not a few compressed actin filaments appear that causes local negative cortical tension even though the overall cortical tension is positive, and temporal variation in cortical tension is happened by co-dynamics of actin, myosin and crosslinker.

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High order methods for time-dependent problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LACUNAE-BASED COMPUTATION OF SINGLE-FREQUENCY SCATTERING VIA TIME-DEPENDENT EMBEDDING

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ABSTRACT

We propose an algorithm for computing the time-harmonic scattering of a scalar field about an obstacle of an arbitrary shape immersed into a homogeneous environment. The algorithm is completely free of any spurious reflections from the artificial outer boundaries. It handles complex shapes not conforming to the discretization grid with no loss of accuracy, contains a reusable core that allows one to change the boundary conditions conveniently and at a low cost, and is easily parallelizable. It is a finite difference algorithm and can employ any standard or high-order accurate scheme. The implementation and error control are straightforward.

The algorithm relies on the method of difference potentials and interpretation of the time-harmonic wave field (solution to the Helmholtz equation) as a solution to the corresponding unsteady wave equation left behind the aft front of the outgoing wave (i.e., solution inside the lacuna of the wave equation).

We demonstrate the performance of the proposed methodology by computing the scattering about a sphere on a Cartesian grid, as well as scattering about a more realistic patch-based configuration built with the help of the CAD software. Extension to the case of a vector Helmholtz equation can also be considered.

Computation for energy storage
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ELECTRO-CHEMO-MECHANICS IN THE APPLICATION OF SOLID STATE BATTERIES

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ABSTRACT

Electro-chemo-mechanics is the relationship between electrical, chemical, and mechanical properties and the study of adjusting one property through the control of another. This relationship can result in special properties for solid-state materials, for instance, the mixed ionic and electronic conductivity (MIEC) of solid electrolytes (SE) in solid-state batteries (SSB). [1] In addition, the ionic and electronic mobility of solid electrolytes can be modified in strained systems (electro-mechanic) [2], and large stresses may be developed in the crystal structure due to non-stoichiometry-induced lattice dilation (chemo-mechanic) [3]. While the origins and characteristics of the electro-chemical relationships have been the focus of many studies, much less is known about the electro-mechanical, chemo-mechanical, and electro-chemo-mechanical relationships.

In this work, we are presenting an electro-chemo-mechanical model which incorporates mixed ionic-electronic conduction for SSBs to describe dendrite propagation in an SE with microstructural defects. A new framework for the metal deposition inside isolated pores of the SE and its coupling with SE fracture is established. The metal deposition in the voids is divided into three stages (metal initiation, metal growth, and metal compression), and the time needed to complete each stage is derived and related to the void size, applied current density, and SE material properties (such as ionic/electronic conductivity and fracture toughness). The electrochemical potentials, deposition overpotential, and current densities of the metal deposition in the void are presented. The deposition-induced pressure and the total time needed for the different stages are quantified. We find that anode voltage, current density, and overall cell potential play a very significant role in determining the vulnerability for metal plating in the SE. Two efficient strategies to reduce/prevent electronic conductivity-driven metal propagation are proposed based on our analysis, including surface coating (or densification) and anode alloying.

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16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Advances in discretization techniques, element technology, mesh adaptivity, and solution strategies for inelasticity, localization, and failure

July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTI-LEVEL OPTIMIZATION-BASED SOLVERS FOR QUASI-STATIC PROBLEMS WITH INSTABILITIES

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ABSTRACT

Many interesting nonlinear mechanics problems can be formulated as constrained optimization problems with non-convex objective functions in the quasi-static limit. Important examples include buckling, fracture and phase transition. Mathematically, these scenarios are characterized by the possible presence of negative eigenvalues in their linearized stiffness matrix. We explore trust-region algorithms which attempt to efficiently identify negative eigenvalue directions using multi-scale information, and which can also utilize a running approximation to the ‘left-most’ eigenvector to further accelerate progress when far away from local minima. When approaching a local minimum, effective preconditioning become essential. Here we use multi-level algorithms which leverage ideas from domain-decomposition and multi-grid preconditioners. We discuss trade-offs between various linear and nonlinear multi-level algorithms for solving these nonlinear equations at scale and give examples involving complex buckling structures.

Scientific deep learning
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SECOND-ORDER SOLVERS FOR TRAINING REGRESSION PROBLEMS IN SCIENTIFIC MACHINE LEARNING

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ABSTRACT

In recent years, we have witnessed the emergence of scientific machine learning as a data-driven tool for the analysis, by means of deep-learning techniques, of data produced by computational science and engineering applications. At the core of these methods is the supervised training algorithm to learn the neural network realization, a highly non-convex optimization problem that is usually solved using stochastic gradient methods. However, distinct from deep-learning practice, scientific machine-learning training problems feature a much larger volume of smooth data and better characterizations of the empirical risk functions, which make them suited for conventional solvers for unconstrained optimization. We introduce a lightweight software framework built on top of the Portable and Extensible Toolkit for Scientific computation to bridge the gap between deep-learning software and conventional solvers for unconstrained minimization. We empirically demonstrate the superior efficacy of a trust region method based on the Gauss-Newton approximation of the Hessian in improving the generalization errors arising from regression tasks when learning surrogate models for a wide range of scientific machine-learning techniques and test cases. We show that the conventional second-order solvers tested, including L-BFGS and inexact Newton with line-search, compare favorably, either in terms of cost or accuracy, with the adaptive first-order methods used to validate the surrogate models.

Advances in damage & fracture modeling of multiphysics materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

UNCERTAINTY QUANTIFICATION OF THE LIFETIME OF SELF-HEALING THERMAL BARRIER COATINGS

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ABSTRACT

Thermal barrier coatings (TBCs) are widely used in jet engines operating at high temperatures to protect the underlying structural components from oxidation and degradation. They consist of a ceramic top coat (TC) layer that is adhered to the substrate with the help of a metallic bond coat (BC) layer. Upon prolonged exposure to thermal cycling, microcracks form and grow slowly parallel to the TC/BC interface, eventually leading to separation and final failure of the TBC. In order to increase its lifetime, a self-healing (SH) TBC composite system has been designed based on including encapsulated healing particles in the top coat near the TC/BC interface. Upon being opened by the passing microcrack, the particles supply a ceramic adhesive that heals the microcracks, thus delaying final failure. To simulate this system, a micromechanical model that incorporates a cohesive-zone based crack healing model was developed, which allows to estimate the lifetime of the TBC upon thermal cycling [1]. Nonetheless, this deterministic model cannot on its own cope with the uncertainties associated to the variability in the micro-structural design variables. In order to consider the uncertainties in input variables, a surrogate model based on a Polynomial Chaos Expansion was developed to emulate the original model in a computationally efficient manner [2]. Variables such as the TC/BC interface amplitude, growth rate of thermally grown oxide layer at the TC/BC interface, diameter and volume fraction of healing particles, and the mean distance of particles from the TC/BC interface were used in the TBC FE model. The trained surrogate model allows to establish the statistical characteristics of the TBC lifetime as well as the sensitivity indices of the input variables. This insight is critical for the design of a robust SH-TBC system in which the role of each parameter is clarified and the variability in the lifetime can be quantified.

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NONLOCAL MODELING OF MACROSCOPIC NON-UNIFORM DEFORMATION INDUCED BY MICROSCOPIC HETEROGENEITY

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ABSTRACT

Engineering materials have microscopic heterogeneity such as a polycrystalline structure in the metallic material, which induces non-uniform deformation in the macroscopic scales when the size differences between macro- and microstructures are small even under macroscopic uniform stress state. In this study, we attempt to directly describe the non-uniform deformation induced by the microscopic heterogeneity and evaluate the development of non-uniform deformation characterized by the interaction between those caused by external factors such as boundary condition and specimen shape and internal factors such as the heterogeneous microstructure.

In the modeling process, the strain distribution obtained from the digital image correlation was used to quantify the non-uniform deformation induced by the microscopic heterogeneity. The average stress-strain relationship is first evaluated based on the distribution of the local equivalent stress and strain. Using the strain calculated using the averaged relationship, we evaluated the strain deviating from the averaged relationship, and they were assumed to be induced by the microscopic heterogeneity of the material. This strain was represented using a constitutive model including the gradient of the plastic compliance, and the parameters employed in the models were fitted using the experimentally measured strain field.

Subsequently, a multiaxial elastoplastic nonlocal constitutive equation was formulated. As the plastic strain field is directly related to the stress field in the proposed method, the nonlocal constitutive equation without an unknown plastic field can be formulated. Finite element (FE) simulations introducing the proposed nonlocal effect indicated that a scale-dependent non-uniform deformation characterized by the interaction between those induced by external and internal factors was predicted.

Phase-field modeling: Analytics, benchmarks, and discussions
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHASE-FIELD SIMULATION OF MORPHOLOGICAL CHANGE AND STABILIZATION OF FOAM STRUCTURE

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ABSTRACT

In this study, foam structure consisting of many separate cells was focused, and its formation and stabilizing process was simulated using phase field model. In a liquid foam formation process, each cell grows spherically before the neighboring cells collide, and then polyhedral shapes are formed. The initial shapes are determined depending on the nuclei distribution, while the cell-shape changes as time passed. The morphological change and the stabilization process were simulated. Multi-phase-field model was used by applying an individual index to each cell, and time evolution was simulated by the finite difference method. As a result, we successfully obtained the expected variation of the foam structure.

OPTIMIZATION OF ULTRASONIC CEREBROVASCULAR STIMULATION THERAPY FOR ALZHEIMER'S DISEASE

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ABSTRACT

In Japan, as the population ages, the number of cases of Alzheimer's disease is increasing. Alzheimer's disease has traditionally been regarded as a disease of the nervous system, but it has been revealed that it is caused by arteriosclerosis due to the deposition of amyloid β in the capillaries of the brain. It has been found that amyloid β is discharged by stimulating cerebral blood vessels with weak ultrasonic waves. Treatment with that method is about to enter Phase 3 clinical trials. Existing devices for other applications are, however, used for brain stimulation, and the sound field used for stimulation has never been optimized. In this study, we propose to uniformly stimulate the brain with a single irradiating plane wave using a transcranial lens. We have already proposed transcranial lenses with appropriately placed point-like scatterers.

Modifying the already developed Monte Carlo method, we attempted to optimize the arrangement of point scatterers so that the incident plane wave ultrasound has a uniform intensity within the brain.
When a plane wave is incident from the front of the skull, however, a remarkable reflection occurs at the back of the head, which cannot be canceled out. In this study, therefore, we propose incidence from the temporal region.

In order to optimize the arrangement of the point scatterer array lens, we minimized the weighted sum of the objective function that makes the ultrasound intensity at each point within the skull a specified value and the objective function that smoothes the sound field intensity. We systematically investigated the smoothing effect by varying the weight of the weight sum. This problem turned out to be much more difficult than optimizing a lens that focuses transcranially into the brain.

This work was supported by JSPS Grant-in-Aid for Scientific Research, Grant Nos. 19H00740 and 22K03987.

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DIGITALIZATION OF MANUFACTURING SYSTEMS BY USING DIGITAL TRIPLET

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ABSTRACT

Digitalization is eagerly required in all domains for increasing added value and decreasing costs including labor costs. In this research, digitalization includes the introduction of IoT (Internet of Things), digital tools, software, and the automatization that reduces manpower. This paper discusses digitalization in the domain of manufacturing systems.
Features of Japanese manufacturing style include high quality of products and continuous improvement of manufacturing systems. Both of them are driven by skilled workers and engineers, who are working together. Inappropriate digitalization may bring about negative side-effects on the features of the Japanese manufacturing style. Namely, inappropriate digitalization may eliminate skilled workers and engineers and, as a result, the company cannot maintain the quality and cost-effectiveness of the product and high productivity of the manufacturing system. Moreover, the digitalization may bring about the stagnation of technological progress of the manufacturing system if the digitalization impedes the continuous improvement.
In order to avoid these problems, this paper proposes a method for digitalizing manufacturing systems based on knowledge and skills of engineers. We have proposed the concept of Digital Triplet [1], which records the process of problem-solving of skilled engineers, models the process, and reuses it. In addition to physical world and cyber world, which constitute the traditional digital twin, Digital Triple consists of intelligent activity world, where engineers solve problems using digital twin. In the framework of D3, a problem-solving process driven by an engineer is modeled as “Generalized Process Model (GPM)” by using the process description language for D3 (PD3). Examples of GPM include design, continuous improvement, and fault diagnosis of a manufacturing system. The main idea of the proposed method is to digitalize a manufacturing system based on GPM. This type of digitalization preserves knowledge and skills of engineers described in GPM. And, since D3 is inherently embedded with the mechanism of continuous improvement, the digitalized manufacturing system based on the proposed method inherits the mechanism of continuous improvement. In this manner, the proposed method solves the above-mentioned two problems.
This paper describes the procedure of the proposed method, which supports a team of field engineers and system engineers to accomplish the digitalization and illustrates an example of practical application of the proposed method.

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Multi-scale, multi-rate damage and fracture: Models, experiments, and simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEDUCTION-INDUCTION INTEGRATED MULTISCALE SIMULATION: DISLOCATION PATTERN FORMATION IN FATIGUE

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ABSTRACT

Fatigue fracture in metal is a major failure mode in industrial mechanical components. While the mechanism of fatigue crack propagation can be understood in the mechanical point of view considering the effect of microstructures and crystal orientations on crack growth, there is still much room for investigations of the mechanism of fatigue crack formation under cyclic loading. As the fatigue crack formation is closely related to dislocation network patterns that emerge as a result of mutual interaction between a number of dislocations [1], it is important to clarify the mechanism of dislocation structure formation under cyclic loading.

The reaction-diffusion equation approach is a method widely used to model the dislocation structure formation. A challenge in the approach is, however, the difficulty in the determination of appropriate parameters in the governing equations because deductive (bottom-up) determination for such a phenomenological model is problematic.

To address this problem, we propose an inductive approach with the machine-learning method to search a parameter set that produces simulation results consistent with experiments [2]. Using a thin film model, we performed numerical simulations for various sets of input parameters to obtain dislocation patterns. The resulting patterns were represented by the following two parameters; the number of dislocation walls, and the average width of the walls. Then, we constructed an artificial neural network (ANN) model to successfully map between the input parameters and the output dislocation patterns. This scheme of inductive approach to scale-bridging enables top-down determination of appropriate constitutive laws of materials.

In addition, we propose statistical atomistic models to estimate coefficients of dislocation diffusion and interaction that appear in the reaction-diffusion equation. This way one can determine the phenomenological model parameters in the bottom-up (deductive) fashion. Combined with the aforementioned top-down approach, a new scheme to bridge models for different length scales, which we call DIMS (deduction-induction integrated multiscale simulation), can be established. This framework employing the two-way determination of model parameters is expected to enhance the reliability of hierarchical multiscale simulation models.

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Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ELASTO-MECHANICAL CHARACTERIZATION OF BIOFIDELIC SOLID-LIQUID COMPOSITES

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ABSTRACT

Biofidelic soft composite materials that mimics the mechanical properties of human tissues have numerous applications ranging from prosthesis development to wearable devices. These composite materials typically comprises of a soft inclusion phase embedded in a soft matrix. In this work, a category of soft composite materials exhibiting biofidelic characteristics with liquid inclusions embedded in a soft matrix called Solid-Liquid Composites (SLCs) are developed [1]. The introduction of a liquid phase, such as water, liquid metals, or complex fluids, into the soft matrix imparts distinct properties and characteristics that may differ from those of pure solids or liquids. The soft and functional nature of SLCs makes them well-suited for use in soft robotics, biomedical applications, sensing devices, flexible electronics, targeted drug delivery systems, impact resistance, and energy dissipation applications. Tailoring the properties of SLCs to specific needs is achievable by controlling the type and volume fraction of the liquid inclusions.

A unique approach to fabricating Solid-Liquid Composites (SLCs) using commercially available soft silicone matrix (Smoothon Ecoflex 00-30) and laboratory-grade liquid glycerin will be discussed [2]. While Eco-flex 00-30 replicates the behavior of a specific class of human tissues, glycerin is selected due to its non-toxic and immiscible properties with silicone. An experimental approach to characterize the elastic properties of the SLCs, followed by the development of linear-elastic based study to understand size-effect of the inclusion phase, and hyperelastic based material models will be discussed.

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Physical models and reduced order models augmentation with data for physics-informed machine learning in real-world applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SINGLE- AND DOUBLE-GENERATOR BRACKETS FOR THERMODYNAMICS-INFORMED NEURAL NETWORKS

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ABSTRACT

The development of neural networks consistent with the laws of thermodynamics can be achieved by imposing inductive biases on the network by defining the problem structure with thermodynamically coherent formalisms such as Poisson brackets. This formalism can be extended to take into consideration dissipative effects in dynamic processes by introducing dissipative brackets and changing the energy generator for a combination of the conservative energy and the entropy. Different approaches can be used as different generators (energy descriptors of the problem) can be defined [1]. By considering a single energy generator, the generalized free energy of the system (a combination of the internal energy and the entropy, i.e., F=E+S), the Single Bracket can be defined. Another option, as in the case of the GENERIC formalism, is to define two separated energy generators corresponding to the conservative energy (E), and the dissipative energy (S) [2].
The differences in the reconstruction of different non-conservative dynamics through the described formalism, Single Bracket (SB) and double bracket or GENERIC (G), have been analyzed in the development of thermodynamics-informed neural networks [3]. Different advantages and limitations have been found in each formulation in data reconstruction.
Even when both formulations are thermodynamically consistent, GENERIC can impose easily thermodynamic restrictions on the system through consideration of the degeneracy conditions in the system. Even though the energy conservation is not explicitly imposed in SB, this is fulfilled to the extent that the network learns the state variables in latent space.
Despite the similarity in the formalisms, the net hyperparameters play different roles in both formulations. As SB formalism depends only on the data training, it increases precision as the available data increases, but it is highly dependent on network capacity. For its part, the degeneracy conditions on G formalism improve the generalization of the problem, providing robustness to the system, limiting the overfitting of the network, and being able to reconstruct the system with less data.

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Scientific deep learning
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GOAL-ORIENTED ADAPTIVITY FOR SOLVING PARTIAL DIFFERENTIAL EQUATIONS USING ARTIFICIAL NEURAL NETWORKS

Carlos Uriarte[1], David Pardo[2], Jamie M. Taylor[3], Victor M. Calo[4] and Ignacio Muga[5]*

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ABSTRACT

Over the last two decades, Goal-Oriented Adaptivity (GOA) has been extensively studied and developed for the Finite Element Method (FEM). It is a technique that consists of enhancing the discretization of the underlying mesh with the aim of approximating a specific Quantity of Interest (QoI) rather than the error in the energy norm [1].

In this work, instead of considering a FEM discretization, we use neural networks. By adopting an Extreme Learning Machine interpretation for feed-forward neural networks [2], we are able to establish a Petrov-Galerkin-type approach such that: (i) the basis functions are no longer locally supported, and thus possess the potential to overcome the curse of dimensionality; (ii) the basis functions are governed by trainable parameters, yielding a highly non-linear scheme; and (iii) for each choice of trainable parameters, the optimal coefficients of the corresponding linear combination are efficiently computable following a minimum residual methodology. In this way, each GOA iteration is identified in our proposal as a training step of neural networks where the loss function represents an appropriate upper bound of the QoI.

We restrict ourselves to symmetric and positive-definite problems to ensure that we can incorporate robust error estimators for the primal and dual problems within the loss function. Extending it to non-symmetric or indefinite problems requires special care, which we plan to address in future work. The numerical experiments conducted in different spatial dimensions demonstrate the effectiveness of our strategy, up to the optimizer performance capacity and the usual numerical integration challenges.

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Fracture, damage and failure mechanics of cementitious materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL MODELING OF ANISOTROPIC DAMAGE BEHAVIOR IN CONCRETE USING GRADIENT ENHANCEMENT OF TENSILE AND COMPRESSIVE INTERNAL VARIABLES

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ABSTRACT

The most basic damage model treats damage as isotropic using a scalar variable to represent the progressive damage evolution. However, in the case of brittle materials like concrete, failure mechanisms are more complex and dependent on the direction of loading and the mutual interactions of microcracks in the structure. An anisotropic damage law using a second-order damage variable is used in the proposed model to get a better prediction of stress response of concrete under multiaxial loading conditions. The finite element implementation of such a damage model results in spurious mesh sensitivities due to softening-induced localization phenomena of the material. To overcome this, a gradient enhancement technique that introduces an internal length scale is utilized in the model. In this method, higher gradients of certain damage-dependent variables are introduced in order to enrich the standard continuum. To account for the asymmetry in the tensile and compressive behavior of concrete, two separate equivalent strains are incorporated as the regularizing or nonlocal variables in the proposed model. These variables are introduced as the nodal degrees of freedom in the finite element system. The model is validated for different experimental results under various load conditions. A few examples are also provided to show the adequacy of the model in the prediction of cracking patterns in concrete structures.

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ENERGY CONSERVATIVE QUADRATURE BASED HYPERREDUCTION OF LAGRANGIAN HYDRODYNAMICS PROBLEMS

Chris Vales[1], Siu Wun Cheung[2], Dylan M. Copeland[2] and Youngsoo Choi[2]*

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ABSTRACT

Dimension reduction methods are used to approximate the numerical discretization of a model in order to reduce the computational cost of its simulation while staying faithful to the full dynamics. To achieve this, projection-based methods construct a reduced basis from full simulation data and project the dynamics onto the spanned linear subspace. For nonlinear problems, hyperreduction methods are additionally needed to remove the dependence of the nonlinear terms on the full problem's size, completing the reduction process. In this work, we develop an energy conservative hyperreduction method for hydrodynamics PDE problems discretized on a Lagrangian moving grid by high order finite element methods [2]. Based on an existing empirical quadrature procedure [3], our method employs sparse numerical quadrature rules to estimate the model's nonlinear integral terms with a chosen degree of accuracy while ensuring that energy is conserved. We apply our method to well established benchmark problems, such as the Sedov blast and Gresho vortex problems [1], demonstrating that it achieves superior energy conservation and similar accuracy and computational speedup compared to the preexisting, non-conservative method.

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Inverse and optimization problems for advanced materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MONOLITHIC FINITE ELEMENT METHOD FOR AN ENERGY-MINIMIZING PHASE-FIELD MODEL OF FULLY EULERIAN FLUID-STRUCTURE INTERACTIONS

Navid Valizadeh[*1], Xiaoying Zhuang[1] and Timon Rabczuk[2]*

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ABSTRACT

In this study, we present a fully monolithic finite element method designed for the simulation of incompressible fluid-structure interaction problems within an Eulerian framework. The fluid dynamics is characterized by the Navier-Stokes equations, while the structural behavior is represented using a hyperelastic neo-Hookean material. The continuum model [1] comprises a system of Navier-Stokes equations coupled with a Cahn-Hilliard phase-field model and an Oldroyd-B type equation. To ensure thermodynamic consistency, forces and fluxes closing the system of equations are derived through energy variation principles. Within this framework, the Cahn-Hilliard model governs the interface position, and the Oldroyd-B equation is utilized to determine the left Cauchy-Green stress tensor, essential for computing elastic stresses within the solid. The solution methodology involves employing a residual-based variational multiscale method for the Navier-Stokes equations, while the Cahn-Hilliard and Oldroyd-B equations are addressed through a mixed finite element method and a standard Galerkin finite element method, respectively. To verify the model formulation and implementation, we conducted simulations for various two-dimensional examples. Furthermore, we expanded the applicability of the method to address frictionless contact problems and three-dimensional scenarios.

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Recent advances in discretization techniques for coupled problems in incompressible fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A CONTINUOUS-DISCONTINUOUS SHALLOW WATER SOLVER FOR COMPOUND FLOOD MODELING

Eirik Valseth[*1], Chayanon Wichitrnithed[1] and Clint Dawson[1]*

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ABSTRACT

Recent tropical cyclones, e.g., Hurricane Harvey (2017) and Hurricane Matthew (2016), have lead to significant rainfall and resulting riverine runoff with accompanying flooding in addition to catastrophic storm surge from the sea. As the interaction between river runoff and storm surge is nonlinear, thus superposition of the two phenomena from separate models is not applicable. Current existing numerical models based on surrogates to the shallow water equation (SWE) incorporate both rain and riverine processes. However, the simplifications make their use limited to inland regions and unsuitable for flow in coastal regions with storm surge. Coastal and storm surge models such as ADCIRC [2], based on continuous Galekrin methods may have issues with mass balance due to their conservation properties. On the other hand, SWE solvers based on discontinuous Galerkin (DG) methods, such as those introduced in [1] avoid these issues due to their local mass conservation property. Recently, we introduced DG solver for a modified SWE for compound flood simulations [3] which incorporated rainfall onto the finite element mesh. In this presentation we explore the use of mixed continuous and discontinuous approximation spaces for the modified SWE to optimize the computational cost. Numerical experiments for past hurricane events will be presented to highlight the capabilities of the proposed scheme and comparison to existing numerical models.

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Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NOVEL SHALLOW WATER EQUATION SOLVER BASED ON MIXED CONTINUOUS-DISCONTINUOUS FUNCTION SPACES

Eirik Valseth[1], Chayanon Wichitrnithed[1] and Clint Dawson[2]*

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[2]The University of Texas at Austin

ABSTRACT

Recent tropical cyclones, e.g., Hurricane Harvey (2017) and Hurricane Matthew (2016), have lead to significant rainfall and resulting riverine runoff with accompanying flooding in addition to catastrophic storm surge from the sea. As the interaction between river runoff and storm surge is nonlinear, thus superposition of the two phenomena from separate models is not applicable. Current existing numerical models based on surrogates to the shallow water equation (SWE) incorporate both rain and riverine processes. However, the simplifications make their use limited to inland regions and unsuitable for flow in coastal regions with storm surge. Coastal and storm surge models such as ADCIRC [2], based on continuous Galekrin methods may have issues with mass balance due to their conservation properties. On the other hand, SWE solvers based on discontinuous Galerkin (DG) methods, such as those introduced in [1] avoid these issues due to their local mass conservation property. Recently, we introduced DG solver for a modified SWE for compound flood simulations [3] which incorporated rainfall onto the finite element mesh. In this presentation we explore the use of mixed continuous and discontinuous approximation spaces for the modified SWE to optimize the computational cost. Numerical experiments for past hurricane events will be presented to highlight the capabilities of the proposed scheme and comparison to existing numerical models.

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Computational methods in environmental fluid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTI-DIMENSIONAL FLOOD MODELING OF AN EXTREME RAINFALL EVENT IN NORWAY

Kristen Valseth[*1], Lars Valnes[1], Eirik Valseth[2] and Kent-Andre Mardal[1]*

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ABSTRACT

Public availability of large high-resolution datasets and advancements in computational capabilities have made the use of partial differential equation based numerical models in hydrology an effective tool for predictions of extreme events and management of water supplies. These developments combined with climate change driven increases in extreme hydrologic events, such as flooding, has generated a need for more accurate and informed water management and prediction tools. As a test case Hans, an extreme storm event in 2023, that saw 100-139 mm of precipitation over a large interior area of Norway in a short time frame was modeled. The event caused widespread damage of infrastructure and property from flooding and landslides, particularly in the area of Nesbyen where the model is focused. To improve future responses and preparation to these types of events this study aims to create more accurate and informed runoff model based on finite element discretizations of surrogates to the shallow water equations. These surrogates include the Diffusive Wave Approximation [1] and the multi-dimensional Kinematic Wave Approximation [2].

In the present work, we develop finite element approximations of these shallow water surrogates. Our focus in the development of a model that utilizes the elevation and landcover data for the Nesbyen catchment and precipitation data from the Hans event as input and model data. Focus is given to the validation of the developed approximations utilizing the diffusive wave model, whereas a novel 1D-2D coupled model utilizing the kinematic wave equation is also presented.

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THEORY OF DESIGN SPACE FILTERING VIA INTEGRAL TRANSFORMS

Hazhir Aliahmadi[1], *Ruben Perez*[2] *and Greg van Anders**[1]

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ABSTRACT

Optimization problems provide some of the earliest, most well-developed, and powerful applications of computation. However, all optimization problems that require significant computation do so because the ultimate, optimal solution cannot be easily deduced from the structure of the problem. Because problem structure—solution structure connections are obscure, it is difficult to understand the relationship between problem and solution features to answer questions about sensitivity, robustness, etc. Here, we describe an integral transformation approach to elucidating the structure of optimization problems. Analogously to the way that integral transforms provide critical insight into problems in signal processing and in control, the integral transform framework we describe here provides new perspectives on the underlying solution space of optimization problems. We show that this framework gives geometric, statistical, and physical perspectives on the form of the solution space of a design problem as a function of the design objectives. We relate the present framework to other known approaches to optimization, some of which emerge as special or limiting cases of the present framework. The framework we present can be applied to a broad range of problems, and we briefly discuss example applications.

Immersed-boundary variational methods: Theory, data structures, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ANALYSIS OF DIVERGENCE-PRESERVING UNFITTED FINITE ELEMENT METHODS FOR THE MIXED POISSON PROBLEM

Christoph Lehrenfeld[1], *Tim van Beeck**[1] *and Igor Voulis*[1]

[1]*University of Göttingen*

ABSTRACT

Geometrically unfitted finite element methods, such as CutFEM, XFEM, or unfitted DG methods, have been developed and applied successfully in the last decades to a wide range of problems ranging from scalar PDEs on stationary domains to systems of PDEs on moving domains and PDEs on level set surfaces. These methods commonly rely on stabilization techniques, for instance, ghost penalty (GP) stabilization to ensure stability independent of the local cut configuration. Mixed finite element methods based on special vectorial finite element spaces, e.g. H(div)-conforming finite element spaces, however, are tailored to preserve conservation properties like mass conversation exactly on the discrete level. By introducing stabilization terms such as GP stabilization, these conservation properties are perturbed. In this work, we introduce and analyse a stable discretization of the unfitted mixed Poisson problem with Dirichlet boundary conditions. Notably, our approach does not require stabilization terms that pollute the mass balance. The key idea is to formulate the divergence constraint on the active mesh instead of the physical domain, which yields a robust discretization independent of the cut configuration without the need for stabilization. This modification does not affect the accuracy of the flux variable and by applying postprocessing strategies to the scalar variable, we achieve optimal convergence rates for both variables and even superconvergence for the scalar variable.

Numerical modeling of granular and multiphase flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COUPLED CALIBRATION FOR COHESIVE AND FREE-FLOWING GRANULAR MATERIALS USING DEM

Marcel van Benten[*1], Dingena Schott[1] and Johan Padding[1]*

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ABSTRACT

Sodium borohydride (NaBH4) is considered as an alternative fuel for the maritime industry [1]. In contrast to conventional fuels, NaBH4 is a granular material. To use a simulation-supported design for assessing the feasibility of equipment designs for storing and handling this material, its mechanical characteristics are required. These are then used to calibrate and verify simulations using the Discrete Element Method (DEM). However, as this is a novel application for this material, virtually no bulk characteristics are known yet. Therefore extensive testing has been done to extract required mechanical characteristics, such as cohesion, adhesion, internal friction, wall friction, and the Angle of Repose (AoR). These experiments showed that NaBH4 is initially free-flowing, but an increase in the moisture content because of an increase in relative humidity leads to an increase in cohesion, effectively reducing the flowability of the bulk material. Furthermore, our experimental results showed plastic deformation of individual NaBH4 particles.

This work focuses on capturing both the free-flowing and cohesive behaviour of NaBH4 in DEM. To this end, the two-step calibration approach introduced by Grima [2] is adopted and adjusted. First, the free-flowing behaviour is calibrated using a non-cohesive contact model, Hertz-Mindlin (HM). Second, the cohesive material is calibrated using the appropriate cohesive parameters of the Edinburgh Elasto-Plastic Adhesion contact model (EEPA), while the (calibrated) non-cohesive parameters are kept constant. The novelty of this work is the use of EEPA for the second calibration step, which allows the modelling of both the cohesive behaviour and the plastic deformation of the individual particles in the bulk material.

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Computational modeling of extreme-loading events
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SIMULATING DYNAMIC MATERIAL EXPERIMENTS USING A LAGRANGIAN CODE IN TWO- AND THREE- DIMENSIONS

Kendra Van Buren[1], Saryu Fensin[1] and Anna Llobet[1]*

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ABSTRACT

Experiments simulated with Lagrangian codes will often try to take advantage of axi-symmetry to model experiments in two-dimensions, thus requiring less computational expense. However, the necessary assumptions break down when simulating experiments with real-life defects or other three-dimensional features. In this talk, I will discuss some recent results for simulating explosively-driven shock experiments used to better understand material behavior undergoing plane-wave shocks. The plane wave shocks used in these experiments result in higher pressures than dynamic experiments such as flyer-plate experiments, which have been routinely used to study material strength. These experiments, known as the "Lens" experiments to describe how the plane-wave shock is generated, were performed at the Proton Radiography (pRad) facility at Los Alamos National Laboratory (LANL) [1]. The experimental data that are used to evaluate the models include experimental velocimetry data and radiographs. The velocimetry data measure how the face of the material sample is accelerated by the plane-wave shock, and the radiographs provide snapshots of the material areal density at discrete timesteps.

The Lens experiments are simulated using FLAG, a langrangian hydrodynamics code developed at Los Alamos National Laboratory, in both two- and three-dimensions. These simulations are performed using conformal meshing and Arbitrary Langrage Euler (ALE) to mitigate mesh tangling issues, and the material behavior is simulated with models for material strength and spall. Efforts have been made to compare both two- and three- dimensional simulation results to experimental data, and results will be presented that compare how the simulation performs in both dimensions. Progress toward simulating defects in the material sample will also be presented, and the presentation will include discussion about how we intend to develop our simulations and future Lens experiments to continue studying material strength and damage behavior.

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Recent advances in high-order methods for computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN IMPLICIT EXTENDEND DISCONTINOUS GALERKIN SHOCK-TRACKING METHOD

Jakob Vandergrift[*1] and Florian Kummer*[1]

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ABSTRACT

We present a new approach for tracking high-order shocks, drawing on ideas from implicit shock tracking (developed by Matthew Zahr et al.) and extended discontinuous Galerkin (XDG) methods tailored for solving partial differential equations (PDEs) characterized by abrupt changes.

Within XDG methods, interfaces like phases in multi-phase flow are sharply represented using level set functions. This locally enriches the approximation space, accommodating additional jumps in the solution. We focus on devising an XDG method specifically for accurately portraying shock fronts in supersonic flows.

At the heart of our method lies a PDE-constrained optimization problem. Here, both the XDG coefficients of the solution and the level set serve as variables. We tackle the iterative computation of shock-aligned solutions using a Sequential Quadratic Programming (SQP) method, reinforced by various measures to ensure robustness.

To validate our XDG shock tracking method, we demonstrate a proof-of-concept through a range of two-dimensional problems. These include the 1D space-time advection equation, 1D space-time Burgers equation, 1D space-time Euler equations, and the steady 2D Euler equations.

Design beyond optimization: Why, what if, and how much?
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LEARNING TO CHOOSE OPTIMIZERS

Martin van der Schelling[*1], Deepesh Toshniwal[1] and Miguel Bessa[2]*

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ABSTRACT

Optimization plays a central role in Computational Mechanics. However, selecting the right optimization algorithm for a particular task is usually not trivial, as that results from the nature of the optimization problem to be solved and constraints such as available resource budget and training data. In order to address this, there has been a transition from creating hand-designed optimization algorithms to learning how to optimize (L2O), i.e. an approach attempting to learn the optimization conditions themselves. While many studies in the field of L2O have demonstrated good performance on a specific task distribution, they often suffer from poor generalization to other distributions. In addition, established L2O methods are often limited to a specific class of optimization algorithms.

We propose a new approach called "Learning to Choose Optimizers" (L2CO). Our method allows a meta-learner to select at test time from a range of static and well-established optimizers, also allowing to switch to a different optimizer during the optimization process itself. This enables the system to adapt to different task distributions and enhance generalization performance. The framework is set up to continuously incorporate new optimization algorithms and problems, inviting domain experts to contribute their insights and expertise for ongoing expansion.

In this study, we train our model offline on a diverse set of benchmark loss-functions and apply a range of gradient-based, population-based, and probabilistic model-based optimizers. The potential of this approach is demonstrated by comparing its performance to classical optimizers and established L2O-architectures on benchmark loss-functions and simple material design studies. The results suggest that L2CO can be a useful tool and exhibits better generalization. Our code and documentation is available as open-source using f3dasm (framework for data-driven design and analysis of structures and materials): https://github.com/bessagroup/f3dasm.

ADAPTIVE MESH REFINEMENT AND COARSENING PROCEDURES FOR THE VIRTUAL ELEMENT METHOD

Daniel van Huyssteen[*1], Felipe Lopez Rivarola[2], Guillermo Etse[2] and Paul Steinmann[1]*

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ABSTRACT

The virtual element method (VEM) is a recent extension of the finite element method that permits arbitrary polygonal element geometry in two dimensions. This mesh flexibility means that the VEM is well-suited to problems involving adaptive mesh refinement. However, the VEM function spaces are defined such that quantities are only explicitly known on element edges. Thus, the well-known approaches to mesh adaptivity developed for finite elements cannot be directly applied to problems involving the VEM.

A simple energy error estimator has been implemented using a super-convergent patch recovery procedure. Using this error estimator elements are flagged for refinement or coarsening. The refinement [1] and coarsening [2] of the elements is performed using novel remeshing procedures that are suitable for the arbitrary polygonal element geometries permitted by the VEM. The remeshing procedures have been implemented for the VEM for the case of two-dimensional elastic problems. The procedures are motivated by seeking to reduce the global error approximation and to improve/smooth the error distribution over a problem domain to improve the efficiency of the VEM approximation. The performance of the remeshing procedures has been investigated in terms of accuracy in the H1 error norm with respect to computational cost and is compared to a traditional reference uniform mesh refinement procedure.

Numerical results over a wide range of benchmark problems demonstrate that the proposed remeshing procedures represent significant improvements in computational efficiency. Specifically, the adaptive refinement procedure generates solutions of equivalent accuracy to the reference procedure while using significantly fewer degrees of freedom, and significantly less run time. While the adaptive coarsening procedure can generate meshes comprising significantly fewer degrees of freedom compared to uniform meshes while introducing only a small amount of error into the approximation. Finally, preliminary results from concurrent refinement and coarsening schemes show great promise.

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Data-driven methods for modeling complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN MODELING OF COMPLEX MECHANICAL COMPONENTS FOR INTEGRATION IN SYSTEM-LEVEL SIMULATIONS

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[3]Flanders Make
[4]University of Washington

ABSTRACT

Mecha(tro)nic systems often incorporate complex nonlinear mechanical elements like bushings and shock dampers for which high-fidelity modeling approaches, such as nonlinear finite element analysis and computational fluid dynamics, offer precise analysis of these components. However, their computational cost often prohibits their inclusion in broader systems-level simulations, particularly for complex industrial systems featuring numerous such components. Conversely, the approximation of these complex components through idealized models and low-fidelity approaches proves challenging, as these models often lack the requisite accuracy, leading to suboptimal analyses of the system's dynamic behavior.

This contribution presents a Neural Network (NN) structure designed to emulate this first-principle modeling approach. The dynamics of physical systems are typically characterized by underlying states (h), often unknown for complex mechanical components, and describable by ordinary differential equations (ODEs). The system typically initiates in a specific state (h0) and can be excited by inputs (x). Engineers seek specific quantities (y), such as forces or accelerations, through a measurement equation (m) that relates these quantities to the system's states (h) and inputs (x).

In the present approach, gated recurrent units (GRUs) are employed to approximate the ODEs describing the system's states over time, followed by a deep feedforward neural network (FFN) mapping these states to a target variable. The networks are shown to predict a latent space capable of modeling the underlying dynamics, without the need for measuring the full state vector and only relying on the target values y and inputs x. Subsequently it is shown that a nonlinear coordinate transformation exists between the latent space of the network and the states obtained from the reference ODE integration (simulation).

To have a verification of the network’s performance, it is applied to simulation-based data of an academic example for which the states and equations are known beforehand. Furthermore, the methodology is also applied to real measurement data from an INSTRON testing system capturing shock damper and bushing dynamic behavior.

Lastly, it is demonstrated that the trained network can be symbolically approximated, resulting in an ODE expression of the dynamics of the latent states, and a measurement equation for mapping the states to the target variable. This feature allows seamless integration of these networks into variable time-step, system-level simulation software.

Physics-based data-driven modeling and uncertainty quantification in computational materials science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HYBRID PHYSICS-NN MODEL FOR DYNAMIC ANALYSIS OF MULTI-COMPONENT SYSTEMS

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ABSTRACT

Dynamic analysis of multi-component systems is a challenging task, as in some systems, a few components can be predominantly inaccessible. It may be impossible to obtain sensor readings or measurement data from these components or subsystems. In more complicated scenarios, even a baseline mechanistic model may not be available for updating these subcomponents. Practical instances of such systems include the support of bridges and the enclosed core of nuclear reactors. This lack of mechanistic detail and relevant measurement data of a subsystem, along with measurement noise, poses a mathematical challenge for system identification. When dealing with such intricate multi-component dynamic systems, relying on physics-based models may yield inaccurate predictions due to model approximation errors and purely data-based models need large amount of training data and may result in predictions inconsistent with physics laws.

To address this challenge, we propose a hybrid approach that blends physics-based and neural network (NN) methodologies for modeling two subsystems. The primary challenges lie in (i) integration of these two approaches --- as there is an interaction between subsystems, and (ii) extraction of the system parameters of the unknown subsystem. Extensive research has been done on combining data driven and physics-based methods. For instance, discrepancy modeling, where the model form error is learned through machine learning techniques [1,2]. In [3], the authors have attempted to learn the interaction force through data-based models.

The novel aspect of this paper is to propose a numerical framework to couple a dynamical system and a neural network when only one subsystem is instrumented and known. It focuses on understanding the modes of interaction, effect of nonlinearities, and the demand on measurement data within this coupling framework. These aspects are studied using a two span beam model, with one span being inaccessible --- leading to uncertainty in the system parameters and boundary conditions. The response of the coupled system subjected to an untested external input, as well as the system parameters, are estimated.

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Multiscale computational and data-driven approach of advanced materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATION OF THE FREE ENERGY PRINCIPLE IN MATERIALS SCIENCE (INTELIGENT MATERIALS AND STRUCTURES)

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ABSTRACT

This paper presents an approach to the design of intelligent materials [1] based on multilevel modeling, the free energy principle and the method of nonequilibrium statistical operator developed by Zubarev [2]. The method of multilevel modeling is based on the postulation of scale levels. For each scale level, a system of structural levels reflecting the real internal organization of a particular material is introduced. The method of nonequilibrium statistical operator is used to construct integral-differential equations at each of the micro- and meso-levels to describe the behavior of an intelligent material and allows us to take into account the dynamic correlations between the material, as an open system, and its environment. The free energy principle is used as a functional to optimize the performance of the material at each of these levels. At the macroscopic scale, the concept of effective material characteristics is used to describe the behavior of intelligent material structure, which are used as input data for finite element modeling in CAE systems. The transition from mesoscale to macroscale is carried out through obtaining effective material characteristics on the basis of periodicity cell investigation. Based on the developed approach, the characteristics of active material components (sensors and actuators) were calculated to control the shape and size stability of the thin-layer structure of the space antenna mirror.

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Numerical modelling of composite materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING OF WOVEN CERAMIC MATRIX COMPOSITES USING AN EMBEDDED FIBERS APPROACH

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ABSTRACT

Ceramic matrix composites (CMCs) exhibit exceptional mechanical properties at elevated temperatures, making them promising candidates to replace metal alloys in high-temperature components of aircraft engines. However, CMCs also exhibit variability due to both their internal structure and the inherent properties of their constituent phases. To better understand and predict their mechanical behavior within the context of this variability, the development of numerical models that capture crucial phenomena at both micro- and meso-scale levels is of paramount importance.

The proposed ”embedded fibers” approach aims to overcome the challenge of scale separation by explicitly incorporating fibers and interfaces at the meso-scale, but without demanding excessive computational burden when compared to direct numerical simulations. Expanding upon previous studies [1, 2], our approach employs a discrete representation of fibers and their interaction with the matrix to faithfully capture the material’s structure and woven architecture. The proposed model is first validated against direct numerical simulations featuring explicitly meshed fibers and cohesive zone models. Virtual tensile tests are then compared with experimental observations to gain deeper insights into microscale mechanisms. Lastly, a parametric study is conducted to evaluate the impact of model parameters on the material’s mechanical behavior and failure characteristics.

The developed approach demonstrates the ability to capture both the micro-scale mechanisms and meso-scale behavior of CMCs, offering a valuable tool for understanding and predicting their mechanical performance in the context of their variability. This work paves the way for further developments towards the optimization of the design and performance of CMC components.

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Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREDICTION OF RESIDUAL STRESSES IN METAL LPBF PARTS THROUGH A HOLISTIC MULTISCALE SIMULATION APPROACH

Yohann Vautrin[*1], Jean-Philippe Marcotte[1], Kalonji Kabaa Kabanemi[1], Marjan Molavi-Zarandi[2] and Florin Ilinca[3]*

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ABSTRACT

Laser Powder Bed Fusion (LPBF) has emerged as a revolutionary additive manufacturing process for the manufacture of complex metallic components, but various challenges still curtail its widespread use by industries. Among these challenges, deformations caused by residual stresses accumulated during printing can lead to severe defects ranging from low geometric accuracy of the as-printed parts to build failure caused by cracking or warpage. Numerical simulation of the LPBF process can help understanding the thermomechanical behavior of a part during printing and predicting its warpage without actually running any costly printing job. In this context, we present a holistic multiscale finite element analysis (FEA) simulation methodology that is able to predict the residual stresses and their associated deformations in metal LPBF parts.

A common obstacle in the numerical simulation of the LPBF process is the number of different spatial and temporal scales involved. While part-scale builds usually have a size in the scale of centimeters and take hours to be built, the laser beam operates on a much smaller scale, typically in the scale of micrometers and the timescale of the order of microseconds. Simulating the entire process at the meso-scale level is not tractable in practice and a multiscale simulation methodology is thus warranted. The continuum approach we have developed involves solving two distinct numerical problems at the meso-scale and at the part-scale levels, respectively.

The meso-scale model is a high-fidelity coupled thermomechanical simulation of the LPBF process that takes into account the dynamics of powder melting and solidification caused by a moving heat source representing the laser beam and its resulting strains and stresses in the material. This problem is solved on a small domain representative of the laser hatch pattern over short time periods (millimeters / seconds) and yields so-called “inherent strains” that are extracted in accordance with the modified Inherent Strain method. The part-scale model uses a layer-by-layer approach, with possible layer lumping, to simulate the LPBF process on full-scale parts. Its simplified physical models give access to the evolution of temperature in the part over the duration of the build and leverages the inherent strains extracted from the meso-scale model to predict the deformations of as-built parts. Our approach will be demonstrated on cantilevers and results will be compared with experimental data.

16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Advances in discretization techniques, element technology, mesh adaptivity, and solution strategies for inelasticity, localization, and failure

July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATIONS OF MESH ADAPTIVITY AND TRANSFERS FOR MODELING FRACTURE AND FAILURE

Michael Veilleux[*1], James Foulk[1], Mark Merewether[1], Matthew Staten[1], Riley Wilson[1], David Noble[1] and Gabriel de Frias[1]*

[1]Sandia National Laboratories

ABSTRACT

Finite element modelers of fracture and failure are frequently constrained by the numerical limitations presented by a single discretization of the domain. A Lagrangian finite element mesh limits the ability to model both large deformations in ductile failure and fragmentation in higher rate brittle failure. Furthermore, the refined, well-structured mesh required for resolution of localization and near-crack fields can be numerically intractable to include in models of entire parts or systems. These limitations can be greatly reduced by the ability to model a problem with multiple meshes, but only with careful consideration of the transfer operation.

This presentation revisits recently implemented finite element technology focused on preserving solutions across transfers and shows multiple applications. These applications include: large-deformation, ductile failure with a sequence of mesh adaptions and transfers; brittle material fragmentation with transfers between Lagrangian meshes and particle meshes; and, computation of high resolution fracture energies along a small, stationary crack in a large body by transferring deformation and stress fields onto a well-structured, templated mesh of the crack.

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ON AN EFFICIENT PARAMETRIC PGD SOLVER FOR DAMPED ELASTODYNAMICS OPTIMIZATION

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ABSTRACT

The talk will focus on a parametric Galerkin-based Proper Generalized Decomposition (PGD) solver for the simulation of damped mechanical structures. The solver builds on recent developments of a space-time PGD solver [1,2] which relies on the Hamiltonian formalism, for the construction of reduced-order models (ROM). Some key ingredients greatly improve the computational efficiency of the classical PGD approach when applied to structural dynamics. The novelty of our approach lies in the design of a solver that is halfway between the Modal Decomposition method and the conventional PGD framework and aims at accelerating the fixed-point iteration algorithm. It essentially consists in pre-processing the eigen-pair approximations of the operators, namely the Ritz pairs, that provide a subspace in which the PGD problem in space remains diagonal throughout the fixed-point iterations. All computations are then carried out in the subspace spanned by the Ritz vectors [3] hence drastically decreasing the computational burden while capturing most of the information from the full model using only a small number of modes. Additional procedures such that Aitken's delta-squared process and mode-orthogonalization are also employed to ensure convergence and stability of the algorithm while progressively computing the new modes.

The methodology has been straightforwardly extended to viscoelastic systems modeled with Rayleigh damping, writing the damping matrix as C=aM+bK, where M and K are respectively the mass and stiffness matrices. It allows for the construction of a parametric ROM with respect to the Rayleigh damping coefficients a and b. Subsequently, the ROM can be used to efficiently identify the damping parameters with respect to given snapshots. The goal is to find the optimal pair (a*,b*) that minimizes the error between the solution of the model and the snapshots. The optimization problem is solved using the Particle Swarm Optimization (PSO) approach in which the pair (a,b) for each particle in the search space is updated in parallel based on the surrogate ROM. The relevance and performance of the proposed approach, namely the ROM accuracy, time complexity, and scalability, will be demonstrated on several numerical examples dealing with three-dimensional structures.

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Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IN HONOR OF PROFESSOR J. TINSLEY ODEN: A UNIFIED PHASE FIELD APPROACH TO ELASTIC-PLASTIC FRACTURE

Kumar Vemaganti[*1], Pietro Pascale[2] and Krishna Kenja[2]*

[1]*Sandia National Laboratories*
[2]*University of Cincinnati*

ABSTRACT

There are few, if any, disciplines within computational science and engineering left untouched by the pioneering contributions of Professor J. Tinsley Oden. Phase field modeling, the idea of capturing sharp changes in the material phase with a diffuse interface, is one such computational approach studied by Professor Oden more than a decade ago [1].

In this talk, we present a unified phase field approach to modeling elastic-plastic fracture. The proposed approach is an extension of the classical variational model of fracture, and can represent a wide range of behaviors, from brittle to ductile, without resorting to phenomenological assumptions. This is achieved by independently modeling the phenomena of plasticity and separation using two phase fields: a slip field to represent plasticity and a damage field to represent cracks.

The slip field seeks to capture plasticity at the meso-scale [2] and extends to the general load case the model of plastic slip presented by Ambrosio et al [3]. The damage field interacts with the slip field by the known phenomenon of pre-localization that is characteristic of some free-discontinuity formulations. Numerical results show that the proposed mesoscopic two phase field model is capable of reproducing a wide range of fracture behaviors, and can be easily correlated to ASTM standard testing results.

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Advances in material model calibration for computational solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN APPROACH TO THE BAYESIAN CALIBRATION OF PHASE FIELD MODELS USING DIMENSIONAL ANALYSIS: APPLICATION TO ELASTOPLASTICITY

Krishna Kenja[1], Pietro Pascale[1] and Kumar Vemaganti[2]*

[1]University of Cincinnati
[2]Sandia National Laboratories

ABSTRACT

Model calibration is a fundamental part of developing and deploying reliable and predictive computational models. A vast amount of literature exits on the topic, but a black-box approach may not always be feasible and considerations based on the nuances of the specific model under investigation are often necessary. This is especially true for phase field models where calibration is a challenging task because of the multiscale nature of problems, non-unique mappings of input parameters to output quantities, and the nature of the regularization length-scale parameter.

In this talk, we present an approach that brings together dimensional analysis, conditional latin hypercube sampling and Bayesian calibration to determine posterior distributions on the parameters for a phase field model. The phase field model under consideration [1,2] seeks to approximate plastic slip lines as degenerated gradients and its response is governed by three parameters: a length scale parameter to regularize the displacement discontinuity across the slip line, an unpinning energy parameter that characterizes the bulk energy density needed to initiate slip, and a gliding resistance parameter that represents the dissipation during sliding along the slip lines. It is known that the model's parameters cannot be calibrated from its macroscale response alone, a manifestation of the Hall-Petch effect.

The proposed approach relies on data from a combination of macro-scale tension tests and meso-scale indentation tests to calibrate the phase field model parameters. Using a series of simulations, we establish relationships between input and output pi groups of the model. These relationships then allow us to calibrate the phase field model. A Gaussian Process (GP) surrogate is used as part of a Bayesian approach to obtain posterior distributions on the phase field model parameters. Our results show that the proposed approach is robust. Equally importantly, we find that the length scale parameter acts both as a numerical parameter and a model parameter for the phase field model under consideration.

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Advances in multi-scale, multi-material, and multi-component Topology Optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION OF MULTI-MATERIAL STRUCTURES VIA TRANSFER-MATRIX NORM MINIMIZATION

*Paolo Venini**[1]

[1]*University of Pavia*

ABSTRACT

The author's group has recently proposed a topology optimization method that is based on the minimization of a suitable norm of the transfer matrix that maps the input to the outputs [1]. The approach is general enough to allow the simultaneous minimization of quantities of engineering interest at the (global) structural level and at the (local) material level in a multi-material framework. For the sake of this paper, multi-material topology optimization shall be exploited with applications to static and dynamic problems. As for the specific applications under investigation, the so called exo-skeleton design problem shall be considered. The idea is to improve the response of existing buildings to horizontal actions, typically of seismic nature, by adding a few exoskeletal structures in strategic locations. Finding the optimal topologies of such kind of structures, as well determining whether a quasi-static idealization may suffice for the scopes, or a dynamic model is needed are among the goals of the paper.

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Enabling technologies for digital twins: Model reduction and scientific machine learning
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

REAL-TIME HIGH-FIDELITY ALGORITHMS FOR EXTREME-SCALE BAYESIAN INVERSE PROBLEMS INVOLVING SHIFT-INVARIANT SYSTEMS

Sreeram Venkat[*1], Stefan Henneking[1], Milinda Fernando[1] and Omar Ghattas[1]*

[1]*The University of Texas at Austin*

ABSTRACT

Tsunamis resulting from megathrust earthquakes have taken the lives of millions and caused hundreds of billions of dollars in damages. To prevent such destruction by future tsunamis, authorities plan to install acoustic pressure sensors on the seafloor to act as an early-warning system. At the core of designing such an early-warning system lies the ability to --- in real-time --- infer the spatiotemporal seafloor deformation from the pressure data and use the inferred deformation to predict the trajectory of a potential tsunami. To this end, we aim to create a digital twin for the Cascadia subduction zone, one of the targeted regions for installing seafloor pressure sensors. The digital twins we target have the following properties: (1) they employ discretizations of high-fidelity PDEs, leading to extreme scale forward problems; (2) they solve an inverse problem to assimilate observational data to infer uncertain model components followed by a forward prediction of the evolving dynamics; (3) the entire end-to-end data-to-inference-to-prediction computation is carried out in real-time through a Bayesian framework that rigorously accounts for uncertainties.

Creating digital twins with the above properties is challenging due to the enormous size and complexity of the high-fidelity models. For example, a reasonable discretization of the Cascadia subduction zone gives rise to a system with O(10^10) parameters and a formal flop count of O(10^30)! Developing accurate and predictive surrogates over a 10^10-dimensional parameter space for tsunami dynamics described by hyperbolic PDEs is seemingly intractable as the PDEs do not admit low-dimensional subspace representations. However, we can circumvent these challenges by exploiting the intrinsic structure of the problem. Namely, our methodology (1) exploits the time shift-invariance of autonomous dynamical systems to reduce the required number of adjoint wave propagations from 10^5 to 100; (2) uses the same property to extract the block Toeplitz structure of the parameter-to-observable (p2o) map; (3) employs FFTs to diagonalize the p2o map; (4) constructs the inverse operator, and thus the posterior precision operator, in the data space rather than the parameter space; (5) decomposes the computation into a more expensive offline phase (done once) and an online phase of inference and prediction that executes in a few seconds; and (6) designs all underlying algorithms to maximize locality, arithmetic intensity, and communication efficiency to run and scale well on large GPU clusters. The result is a framework for extreme-scale, high-fidelity Bayesian inference and posterior prediction in real-time, with application to tsunami early warning.

UQ-TTA student paper competition in uncertainty quantification
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

REAL-TIME HIGH-FIDELITY ALGORITHMS FOR EXTREME-SCALE BAYESIAN INVERSE PROBLEMS INVOLVING SHIFT-INVARIANT SYSTEMS

Sreeram Venkat[*1], Stefan Henneking[1], Milinda Fernando[1] and Omar Ghattas[1]*

[1]*The University of Texas at Austin*

ABSTRACT

Tsunamis resulting from megathrust earthquakes have taken the lives of millions and caused hundreds of billions of dollars in damages. To prevent such destruction by future tsunamis, authorities plan to install acoustic pressure sensors on the seafloor to act as an early-warning system. At the core of designing such an early-warning system lies the ability to --- in real-time --- infer the spatiotemporal seafloor deformation from the pressure data and use the inferred deformation to predict the trajectory of a potential tsunami. To this end, we aim to create a digital twin for the Cascadia subduction zone, one of the targeted regions for installing seafloor pressure sensors. The digital twins we target have the following properties: (1) they employ discretizations of high-fidelity PDEs, leading to extreme scale forward problems; (2) they solve an inverse problem to assimilate observational data to infer uncertain model components followed by a forward prediction of the evolving dynamics; (3) the entire end-to-end data-to-inference-to-prediction computation is carried out in real-time through a Bayesian framework that rigorously accounts for uncertainties.

Creating digital twins with the above properties is challenging due to the enormous size and complexity of the high-fidelity models. For example, a reasonable discretization of the Cascadia subduction zone gives rise to a system with O(10^10) parameters and a formal flop count of O(10^30)! Developing accurate and predictive surrogates over a 10^10-dimensional parameter space for tsunami dynamics described by hyperbolic PDEs is seemingly intractable as the PDEs do not admit low-dimensional subspace representations. However, we can circumvent these challenges by exploiting the intrinsic structure of the problem. Namely, our methodology (1) exploits the time shift-invariance of autonomous dynamical systems to reduce the required number of adjoint wave propagations from 10^5 to 100; (2) uses the same property to extract the block Toeplitz structure of the parameter-to-observable (p2o) map; (3) employs FFTs to diagonalize the p2o map; (4) constructs the inverse operator, and thus the posterior precision operator, in the data space rather than the parameter space; (5) decomposes the computation into a more expensive offline phase (done once) and an online phase of inference and prediction that executes in a few seconds; and (6) designs all underlying algorithms to maximize locality, arithmetic intensity, and communication efficiency to run and scale well on large GPU clusters. The result is a framework for extreme-scale, high-fidelity Bayesian inference and posterior prediction in real-time, with application to tsunami early warning.

Computational fluid dynamics (CFD) and fluid-structure interaction (CFSI): Methods and Applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TURBULENCE MODELING OF HIGH-SPEED FLOWS USING FINITE ELEMENT BASED STABILIZED FORMULATION AND SPALART-ALLMARAS MODEL

Rahul Verma[*1], David Codoni[2], Craig Johansen[1] and Artem Korobenko[1]*

[1]*University of Calgary*
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ABSTRACT

This study involves modeling of high-speed flows using a finite element based stabilized framework along with standard Spalart-Allmaras (SA) model [1]. The set of Navier-Sokes equations for compressible flow in thermal equilibrium is formulated in pressure-primitive variables and Streamline Upwind Petrov-Galerkin (SUPG) method with Discontinuity Capturing (DC) operator are used for stabilization. The formulations was originally proposed in [2]. For time integration the second-order accurate generalized-α method is used. Equations of SA model includes a non-viscous destruction term which relies on the distance to wall. Unlike to the old one equation models, in this model the solution depends on other points of the domain, enabling it to be flexible for all types of grid. Moreover, SA model has proved to be effective in capturing the smooth transition of flow from laminar to turbulent and boundary layers developed at the wall surface. This research focuses on modeling the effects of turbulence on benchmark 2D NASA flat plate case at Mach 2 and Mach 5. Moreover, this study is also extended to analyse a 3D ONERA M6 wing transonic case. The results obtained using present methodology are in strong correlation to the experimental results for both 2D and 3D case. The accuracy of results strongly reflects the stability of the present numerical formulation.

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Continuum biomechanics of active systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN INTEGRATED APPROACH OF EMBEDDING VASCULATURE FOR ANALYSING IN-VIVO TESTING OF THE HUMAN BRAIN

Yashasvi Verma[*1], Emma Griffiths[1], Jakob Schattenfroh[2], Camilla Belponer[3], Alfonso Caiazzo[4], Ingolf Sack[2], Silvia Budday[1], Luca Heltai[5] and Paul Steinmann[1]*

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ABSTRACT

Upon reviewing existing literature, it becomes evident that human brain tissue exhibits conflicting material responses under diverse testing modalities. This inconsistency underscores the necessity for a predictive computational model capable of reconciling these disparate findings. A crucial stride in this endeavour involves the integration of the vascular structure into a continuum material model, aiming to address the coupling dynamics between solid and fluid phases within the tissue. This integration holds the potential to elucidate variations observed between in vivo and ex vivo experimental responses.

The incorporation of blood vessels into the linear viscoelastic tissue is grounded in the multiscale immersed method [1]. In this approach, blood pressure is factored into the forcing term, and a multidimensional coupling is implemented using the Reduced Lagrange multiplier method.
Expanding our model to replicate the magnetic resonance elastography (MRE) test setup, we note previous MRE findings that highlight the influence of blood flow on in vivo brain viscoelasticity [2]. MRE enables the extraction of cerebral mechanical parameters across multiple length scales, both ex vivo and in vivo, spanning the entire brain and various anatomical regions. A comparative analysis between the computational model and MRE data emphasizes the importance of integrating vasculature into the brain computational model, particularly when dealing with in vivo and non-invasive experimental setups.

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FULL WAVEFORM MODELING IN SEISMIC EXPLORATION BASED ON A DIGITAL GEOLOGICAL MODEL USING SPECTRAL ELEMENT METHOD ON GPU

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ABSTRACT

The presentation considers the solution of a three-dimensional problem of modeling of all types of seismic waves propagating in real geological environments [1]. The numerical algorithm based on the spectral element method (SEM) [2]. The main advantages of SEM (high order space discretization, explicit time integration scheme) are presented in comparison with the classical approach based on the finite element method (FEM). The features of the massively parallel implementation of the algorithm on modern MultiGPU systems (based on A100 GPU) using CUDA technology are considered. The efficiency of parallelization on hybrid systems with different SEM orders and parameters of the numerical time integration scheme is analyzed. The results of solving a three-dimensional problem of modeling the propagation of seismic waves in a heterogeneous geological environment with faults and sharply varying properties of layers are presented. Analysis of the numerical convergence of SEM for dispersive waves of the Rayleigh type is performed. Local and non-local non-reflective boundary conditions on the artificial boundary of the computational region are considered.

The 3D computational model is constructed using a detailed digital geological model built for one of the Arctic regions. It was converted to an unstructured hexahedral mesh to perform SEM calculations using CAE FIDESYS software [3]. The model is further generalized for typical seismic-geological conditions of Western Siberia, so that on the basis of such modeling it is possible to conduct a wide range of studies on the possibilities of seismic exploration to study the main oil and gas reservoirs in this region. The solution was sought on a hexahedral mesh consisting of 5.5 mln spectral elements of the 5th order with a total number of SEM nodes 1.2 billion. The output results of full-wave modeling are stored in the SEG-Y format, suitable for all types of industrial seismic processing. The analysis of the obtained model seismograms and wave fields is carried out. The conclusion is made about the practical significance of the conducted research.

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Current trends in phase-field modeling and computations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ON THE ENERGY DECOMPOSITION IN VARIATIONAL PHASE-FIELD MODELS FOR BRITTLE FRACTURE UNDER MULTI-AXIAL STRESS STATES

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ABSTRACT

Phase-field modelling of fracture is gaining popularity in the fracture mechanics community, particularly for its ability to generate cracks with arbitrarily complex geometries and topologies in two and three dimensions without the need for ad hoc criteria. The model first introduced in [1] has a clear connection with Griffith's propagation criterion via Gamma convergence tools and recent results [2] have shown that, in addition to propagation, it can quantitatively predict crack nucleation for mode-I loading. However, the initial model cannot reproduce with flexibility the experimentally measured strengths under multiaxial loads. Moreover, a modification is necessary to avoid the interpenetration of crack surfaces in compression and reflect the physical asymmetry of fracture behaviour between tension and compression [3].

In this presentation, staying within the realm of variational approaches, we discuss existing modifications based on energy decomposition, their shortcomings, and the requirements for an effective energy decomposition method to model crack nucleation and propagation. Finally, we introduce a new energy decomposition, the star-convex model, that solves (at least partially) the issues with the existing ones.

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Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ON THE SOLUTION OF UNSTABLE FRACTURE PROBLEMS WITH NON-LINEAR COHESIVE LAWS

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ABSTRACT

The existence of numerical problems related to damage and fracture models is well-known and documented in the literature. In an implicit finite element formulation, the radius of convergence of the Newton-Raphson algorithm reduces to zero in the presence of unstable solution branches. One of the following instabilities may arise: snap-through under load-control or snap-back under displacement-control. In [1], the authors state that these numerical difficulties occur when the internal energy stored in the bulk material is higher than the amount of energy that can be dissipated through crack initiation and propagation. Additionally, the rate at which these energies increase as the size of a sample grows varies, meaning that these challenges are fundamentally tied to the length scale of the problem.

Although this finding has been mainly reported for linear softening traction-separation laws, this work comprehensively explores non-linear softening behaviours and proposes a more general instability criterion [2]. It is demonstrated that, to cope with quasi-brittle or plateau softening behaviours, the criterion has to be formulated in terms of power or energy rate (in temporal terms) instead of total energy. Accordingly, the ratio of cohesive to internal power emerges as a crucial factor. As a result, even scenarios involving a single cohesive element undergoing monotonic loading may exhibit a limit point at any stage of crack propagation, not just during crack initiation.

Furthermore, two strategies for handling fracture problems with instabilities within an implicit solution are discussed: an arc-length technique and an extension of quasi-static formulation into a dynamic regime. A comparative assessment is performed, covering both simple single-element cases and more complex scenarios. Additionally, the study delves into more intricate material responses, including transformation-induced plasticity effects.

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INPUT-OUTPUT REDUCED ORDER MODELING FOR PUBLIC HEALTH INTERVENTION EVALUATION

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ABSTRACT

In recent years, mathematical models have become an indispensable tool in the planning, evaluation, and implementation of public health interventions. Regardless of specific mathematical formulation, models must provide detailed information for many distinct levels of population stratification. Such detail comes at a price: in addition to the obvious high computational costs, the number of input parameters and outcomes of interest often number well into the tens of thousands. This leads to difficulty at all stages of the modeling workflow: effective study designs can be difficult to develop and computationally demanding; optimization algorithms are slow to converge, and, due the high number uncertain input parameters, may exhibit (perhaps infinitely) many local solutions. Post-processing of model outputs is also challenging, as the large number of outputs can be difficult-to-interpret, and drawing concrete, actionable conclusions and recommendations from simulation results is not necessarily straightforward. While dimension-reduction techniques often show a low-rank structure in the output space, this is of limited utility for intervention planning as connecting the reduced-order outputs to the input space (the relevant space for intervention planning) is difficult.

In this presentation, we focus on addressing these difficulties. We employ polynomial chaos expansion (PCE) to surrogate our full-scale model over a sparse hypercube of model parameter ranges. We demonstrate that this representation enables for fast and effective uncertainty quantification and sensitivity analysis, allowing us to easily identify important model parameters. This has immediate application in study design, as it allows us to reduce the number of exploratory variables.

We then further show that these techniques can also be employed on a reduced-order output space, and that the sensitivity of reduced-order outputs to specific model inputs can be easily assessed. We then further exploit the structure and regularity of the PCE representation to rigorously map the reduced output-space to a corresponding reduced-order input space with low computational cost, allowing us to associate each reduced-order output with a corresponding reduced-order input. We show this representation allows for fast and effective intervention planning with a minimal loss of information and further, that the reduced-order representations of both the input and output spaces are highly interpretable. While we use our HOPE compartmental model for HIV transmission and disease progression as our working example, the principles and techniques discussed also apply more generally.

Multiscale methods for advanced manufactured materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MULTISCALE LAMINATE-BASED MODEL FOR SEMI-CRYSTALLINE POLYMERS

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ABSTRACT

Semi-crystalline polymer morphology is heterogeneous, hierarchical, and complex. At the microscopic level, there is a crystalline phase, often organized into lamellae, embedded in an amorphous phase. In turn, these lamellae commonly organize into spherulites., approximately spherical arrangements of lamellae [1]. To some degree, all these features contribute to the mechanical response of semi-crystalline polymers. Several authors try to capture some of the effects evident in these experimental results by solely considering the volume fraction of the two phases while neglecting additional information regarding the microstructure of these polymers, e.g., [2]. However, to better understand the microstructure evolution of the polymer and its influence on the macroscopic behavior of these materials, we need to include a more adequate description of the polymer's morphology. Accordingly, various authors propose multiscale formulations that take into account the lamellar nature of the crystalline phase, e.g., [3].
In these models, they consider as phases an appropriate number of simple laminates, reflecting the lamellar structure of semi-crystalline polymers, and obtain the macroscopic behavior of the polymer through homogenization. In particular, mean-field averaging is used, where local-global interaction laws replace real interactions between domains. At the microscopic scale, appropriate constitutive laws describe the two constituents.

This work also considers the lamellar microstructure of semi-crystalline polymers, but it does so in an alternative way.
Instead of selecting a priori some number of simple laminates as the relevant phases to represent the microstructure, their appearance follows from an appropriate decomposition of the RVE domain, followed by the application of a dilute or self-consistent local-global interaction scheme.
This approach enables us to make a more informed choice regarding the number and direction of simple laminates to consider in the homogenization procedure, resulting in efficiency and accuracy improvements.
We discuss the continuum formulation, and its computational implementation, and then present a few numerical results.
We explore the local-global interaction laws selected and the impact of the appropriate choice of the number and direction of simple laminates considered in the accuracy and efficiency of the model.

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Trustworthy multi-fidelity and data-driven models for computational applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NON-LINEAR ENCODING FOR MULTI-FIDELITY NEURAL NETWORK SURROGATES

Cristian Villatoro[*1], Gianluca Geraci[2] and Daniele Schiavazzi[1]*

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ABSTRACT

The construction of accurate surrogates is a key step in many outer loop tasks, like uncertainty quantification (UQ) and optimization. Neural Networks (NNs), thanks to their expressiveness, have demonstrated great potential to significantly improve the quality of emulators, particularly in high dimensions. Unfortunately, it is recognized that NNs usually require large amounts of data to be reliably trained and to produce satisfactory prediction accuracy. Recently, multi-fidelity approaches have been proposed to tackle this challenge, creating larger datasets leveraging data sources of varying accuracy and computational cost. Using such approaches it is possible, in principle, to leverage larger training datasets to meet required accuracy thresholds for high-fidelity predictions, all while keeping the overall computational cost below to a predetermined budget. In recent work [1], the correlation between data sources is used as the main mechanism to enhance training accuracy in scenarios of limited high-fidelity data availability. Therefore, the performance of such approaches may degrade for realistic applications where the correlation between model outputs could be low as a result of an inconsistent formulation. To this end, in our recent work [2,3], we show that even a simple linear transformation on the inputs can greatly increase the correlation between high- and low-fidelity models while giving a natural way to resolve differences in model parameterization. In the proposed work, we extend linear encoding [2,3] to non-linear encoding and multiple low-fidelity sources, demonstrating their benefits on multiple test cases, including numerical examples and problems inspired by realistic applications.

[1] Meng, X., and Karniadakis, G. E., “A composite neural network that learns from multi-fidelity data: Application to function approximation and inverse PDE problems,” Journal of Computational Physics, Vol. 401, 2020, p. 109020.
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UQ-TTA student paper competition in uncertainty quantification
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NON-LINEAR ENCODING FOR MULTI-FIDELITY NEURAL NETWORK SURROGATES

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ABSTRACT

The construction of accurate surrogates is a key step in many outer loop tasks, like uncertainty quantification (UQ) and optimization. Neural Networks (NNs), thanks to their expressiveness, have demonstrated great potential to significantly improve the quality of emulators, particularly in high dimensions. Unfortunately, it is recognized that NNs usually require large amounts of data to be reliably trained and to produce satisfactory prediction accuracy. Recently, multi-fidelity approaches have been proposed to tackle this challenge, creating larger datasets leveraging data sources of varying accuracy and computational cost. Using such approaches it is possible, in principle, to leverage larger training datasets to meet required accuracy thresholds for high-fidelity predictions, all while keeping the overall computational cost below to a predetermined budget. In recent work [1], the correlation between data sources is used as the main mechanism to enhance training accuracy in scenarios of limited high-fidelity data availability. Therefore, the performance of such approaches may degrade for realistic applications where the correlation between model outputs could be low as a result of an inconsistent formulation. To this end, in our recent work [2,3], we show that even a simple linear transformation on the inputs can greatly increase the correlation between high- and low-fidelity models while giving a natural way to resolve differences in model parameterization. In the proposed work, we extend linear encoding [2,3] to non-linear encoding and multiple low-fidelity sources, demonstrating their benefits on multiple test cases, including numerical examples and problems inspired by realistic applications.

[1] Meng, X., and Karniadakis, G. E., “A composite neural network that learns from multi-fidelity data: Application to function approximation and inverse PDE problems,” Journal of Computational Physics, Vol. 401, 2020, p. 109020.
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Next-generation numerical methods for coupled multiphysics problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NONLINEAR REDUCED ORDER MODELING OF A MULTISCALE MODEL FOR MICROCIRCULATION

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ABSTRACT

Multiphysics mathematical models of the vascular microenvironment assess the impact of microcirculation in transport phenomena through the tissue. Since the embedded vascular network is characterized by high complexity and multiple scales, the numerical solutions of high-fidelity models are often computationally expensive. We present an alternative strategy that is applied to a 3D-1D computational model for microcirculation [1], based on parametrized partial differential equations. The full order model (FOM) describes blood flow and oxygen transfer from the microvasculature to the tissue and it consists of a 3D model for the tissue combined to a 1D model in the vascular network. We propose a multiscale strategy, decomposing the 3D domain of interest in small voxel components, where local numerical solutions are retrieved. We exploit non-intrusive and nonlinear reduced order models (ROMs) [2] to approximate the parametric map to derive an approximated solution in each voxel. We leverage on proper orthogonal decomposition (POD) methods and we rely on sparse Mesh-Informed Neural Networks [3] to handle the spatial dependencies in the solutions and in the geometrical input data encoding the small scale features of the problem. The adopted ROM is built in a supervised learning framework, hinging on local finite-element approximations. Firstly, it approximates the POD reduced basis coefficients using a neural network that combines dense layers for the physical parametrization with a MINN for the geometrical inputs. Then, a closure model based on the geometrical parametrization is added to augment the first approximation, acting as a fine-scale corrector that retrieves the nonlinear information associated to the high frequencies of the problem in each subdomain. We exploit this result to improve classical homogenization methods for multiscale modeling that neglect smaller scales and capture only the global behaviour in the voxel. Finally, the multiscale simulation is performed deriving suitable multiscale basis functions to assemble the local ROM approximations, solving the multiphysics macro-problem with the embedded complex microstructure.

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Multi-scale modeling and upscaling for flow induced vibrations, from local reference simulations to certified industrial tools
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FLUID-STRUCTURE INTERACTION SIMULATIONS AND MULTI-SCALE APPROACHES FOR NUCLEAR REACTOR APPLICATIONS.

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ABSTRACT

Different fluid-structure interaction (FSI) configurations can be encountered in the frame of nuclear reactors. In this presentation, examples of single-phase cross-flow and axial flow local scale (i.e., CFD) FSI numerical simulations are presented and discussed. The configurations simulated consist of experimental campaigns, for which flow (velocity, pressure) and structure (displacement, acceleration) parameters were measured: this allowed to assess the consistency of the numerical set-up and results, a necessary step towards a comprehensive validation of the numerical simulations. The impact of the numerical treatment of turbulence (linear-viscosity models, second-order models or scale-resolving approaches) is discussed: regardless of the configuration, scale-resolving approaches are found to be required to calculate consistent force spectra. The impact of the numerical schemes, of the retained coupling algorithm, of the system damping and other numerical parameters on the calculated results and on the numerical stability is analyzed. Reduced-order models for the finite element simulation of slender structures are assessed and are found to represent an interesting compromise in terms of precision and CPU requirements.

Typical components of nuclear power plants include a huge number of slender structures, such as tubes and rods. It follows that the study of FSI at the local scale is feasible only for limited portions of the systems. A multi-scale approach for such problems is necessary if one aims at applying an FSI analysis at the industrial scale (which represents the final goal). In such approach, porous media simulations can be employed to calculate the average hydraulic (i.e., the fluid flow) system-scale behavior. These component-scale results can provide numerical boundary conditions to apply to local-scale analysis: this allows to zoom over specific regions, where the FSI can be taken into account by the simulation. Nevertheless, the switch from component-scale to more local scales is far from straightforward: parameters such as turbulence intensity and time/length scales are required to apply consistent boundary conditions at the CFD-scale, and are not directly available from component-scale analysis. A discussion of a R&D work plan on multi-scale strategy for FSI in a nuclear reactor core and on possible methods to face down-scaling issues is proposed.

Machine learning for large scale models in physics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A REDUCED ORDER MODEL CONDITIONED ON MONITORING FEATURES FOR ESTIMATION AND UNCERTAINTY QUANTIFICATION IN ENGINEERED SYSTEMS.

Konstantinos Vlachas[*1], Thomas Simpson[1], Anthony Garland[2] and Eleni Chatzi[1]*

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ABSTRACT

Reduced Order Models (ROMs) form essential tools in various engineering domains by their function as surrogates for computationally intensive digital twinning simulators.
While data-driven reduction processes exist, physics-based approaches can render ROMs interpretable. However, such techniques typically face challenges when dealing with models that feature multi-parametric dependencies, while further requiring a reliable quantification of estimation confidence. The performance of the ROMs is usually tied to the approach employed in associating the defining parameters' vector with an appropriate local reduction basis. We propose using Conditional Variational Autoencoders (CVAEs) to continuously map the required reduction bases to the parameter vector while additionally allowing for a probabilistic assessment of the predicted Quantities of Interest. A main novelty of this work lies in linking the operational space of the ROM to practical features that are automatically inferred from measurements of monitored systems rather than physics-based, and usually a priori unknown, system parameters. An auxiliary task using a feed-forward neural network is introduced to re-establish the required connection to the physical model parameters. Its prediction is treated as the mean of a suitable distribution, while an additional network is jointly trained using the respective probability density function to estimate the uncertainty involved. In this context, we here propose a generative physics-based ROM, able to quantify the confidence involved in its post-deployment estimations while being conditioned to online delivered sensing-based features. These components contribute to developing a generalized representation, offering significant utility for tasks related to Structural Health Monitoring (SHM). A series of case studies are used for validation featuring damage in the form of stiffness reduction or plasticity/hysteresis under multi-parametric dependencies relating to the system's properties and the traits of the input load.

Data-driven modeling and design of materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A LARGE LANGUAGE MODEL AND DENOISING DIFFUSION FRAMEWORK FOR TARGETED DESIGN OF MICROSTRUCTURES WITH COMMANDS IN NATURAL LANGUAGE

Nikita Kartashov[1] *and Nikolaos Napoleon Vlassis**[1]

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ABSTRACT

Microstructure's crucial impact on macroscopic properties is widely recognized, with alloy phase distribution affecting mechanical properties, microfeature precision in MEMS dictating device performance, and cellular arrangement in tissue-engineered scaffolds influencing cell growth and differentiation, among countless other domains of study. While advanced ML-based design and generative AI tools exist to explore the forward and inverse relationships between microstructure and macroscopic behaviors, a substantial knowledge and expertise barrier limits their accessibility and broader application in the field. To address this, we introduce a framework that combines Large Language Models (LLMs) and Denoising Diffusion Probabilistic Models (DDPMs) to streamline the design of complex microstructures for users of all expertise levels in mechanics, materials science, and machine learning. By leveraging LLMs, our framework reduces the expertise barrier, allowing users with diverse backgrounds to specify design objectives in intuitive language. The core of this system is an LLM that interprets these inputs, translating them into actionable directives for a DDPM algorithm. This integration effectively democratizes access to complex design processes, making advanced microstructure design more accessible and adaptable. Central to our methodology are DDPMs, generative models that learn to reverse a Markov diffusion process and have been proven to work exceptionally well in text-conditional settings, enabling the generation of synthetic microstructures with specific, fine-tuned properties. This approach allows the manipulation of microstructure topology within the latent space of the training data, ensuring the generation of realistic and viable designs. Demonstrated using the Mechanical MNIST dataset as a benchmark and extending on the work by Vlassis et al, 2023, our framework highlights the capability of DDPMs in performing the inverse design of microstructures with specific nonlinear properties and in understanding the nonlinear structure-property relationships through natural language commands embedded by the coupled LLM. This is critical for exploring the complex interactions among geometry, topology, and macroscopic properties in materials through a user-friendly text interface. This integration of LLMs and DDPMs aims to introduce a paradigm in microstructure design, combining advanced generative machine learning methodologies under a singular, intuitive interface.

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Lattice Boltzmann modelling and study of complex flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPARISON OF FULLY RESOLVED AND UNRESOLVED PARTICULATE FLOW SIMULATIONS USING THE LATTICE BOLTZMANN METHOD

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ABSTRACT

Particulate flows are ubiquitous in nature and industry and numerical simulations are an important tool to understand them. Fully resolved methods are the gold standard in terms of accuracy, but their computational cost makes studying large problems involving many particles prohibitively expensive. Unresolved methods lessen the computational burden by allowing a mesh size larger than the size of the particles at the price of reduced accuracy. In this study we compare fully-resolved and unresolved methods to simulate particulate flows.

We have implemented a coupled lattice Boltzmann and Discrete Element Method solver that is capable of both fully resolved and unresolved simulations of particulate flows in arbitrarily complex geometries. The implementation is parallelized using MPI which allows us to simulate large problems. The fully resolved method is based on the Momentum-Exchange method [1] in which the no-slip boundary condition on the particle surface is explicitly modelled. The unresolved method is based on an LBM implementation of the Volume-Averaged Navier-Stokes (VANS) equations [2].

We investigate the degree to which unresolved simulations can predict the effect of particles on macroscopic quantities like the pressure drop over a porous medium and the rheology of a sheared suspension. We do this by comparing to both the fully resolved method as well as to popular empirical relations. We show how incorporation of the solid volume fraction in the unresolved model is necessary to obtain realistic pressure drops. Regarding suspension rheology, the essential role of short-range hydrodynamic (lubrication) interactions is highlighted. These are naturally accounted for in the fully resolved model, but must be added through a correction term in the unresolved model to obtain realistic values for the apparent viscosity.

Furthermore, we compare the predicted group dynamics of particles using the fully resolved and unresolved methods. First the drafting-kissing-tumbling phenomenon of two interacting sedimenting particles is simulated. Both the fully resolved and unresolved methods reproduce the characteristic dynamics qualitatively. Our ongoing work concerns the capability of the unresolved methods to predict the behavior of larger groups of sedimenting particles in a Rayleigh- Taylor instability.

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Advanced numerical techniques for fluid flow in porous media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ROBUST SCALABLE FINITE VOLUME METHOD FOR TWO PHASE FLOW THROUGH POROUS MEDIA USING A NONLINEAR COMPLEMENTARITY PROBLEM APPROACH

Naren Vohra[*1], Konstantin Lipnikov[1] and David Moulton[1]*

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ABSTRACT

Multiphase flow through porous media is integral to many applications in geosciences, including oil recovery and carbon sequestration. The governing system of equations presents strong nonlinearities due to advection and solute miscibility, which is accounted for using Henry's law. A popular discretization approach is the use of finite volume schemes, however the presence of nonlinearities requires the use of an appropriate robust solver. In this talk, we present various fully implicit finite volume schemes for two phase flow through porous media using the novel approach of nonlinear complementarity problem (NCP) to handle phase transitions. We consider the linear two point flux approximation (TPFA) to compute the numerical fluxes, and demonstrate the robustness of the semismooth Newton's method as a solver for the nonlinear discrete system. The advantages of the NCP approach over the widely used primary variable switching approach include computational efficiency and increased robustness of the solver, and the choice of TPFA provides an ease of implementation and monotonicity of the solution. We also investigate the effectiveness of appropriate preconditioners, such as ILU and MGR, and provide results on the scalability of our nonlinear solver using physical examples, including the well-known MoMas benchmark problem of gas phase appearance and disappearance. We further discuss the assumptions frequently used in the model equations, such as the existence of the solvent in liquid phase alone with negligible solute concentration, the challenges associated with the extension of the system to three phase flow, and the coupling of multiphase processes in matrix and fracture networks.

Mechanobiology of cells, vesicles and biomembranes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

WRINKLING OF FLUID DEFORMABLE SURFACES

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ABSTRACT

Wrinkling instabilities of thin elastic sheets can be used to generate periodic structures over a wide range of length scales. Viscosity of the thin elastic sheet or its surrounding medium has been shown to be responsible for dynamic processes. While this has been explored for solid as well as liquid thin elastic sheets we here consider wrinkling of fluid deformable surfaces, which show a solid-fluid duality and have been established as model systems for biomembranes and cellular sheets. We use this hydrodynamic theory and numerically explore the formation of wrinkles and their coarsening, either by a continuous reduction of the enclosed volume or the continuous increase of the surface area. Both lead to almost identical results for wrinkle formation and the coarsening process, for which a universal scaling law for the wavenumber is obtained for a broad range of surface viscosity and rate of change of volume or area. However, for large Reynolds numbers and small changes in volume or area wrinkling can be suppressed and surface hydrodynamics allows for global shape changes following the minimal energy configurations of the Helfrich energy for corresponding reduced volumes.

Modeling and learning of structured dynamical systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

POSITIVE REAL BALANCED TRUNCATION MODEL REDUCTION OF MECHANICAL SYSTEMS

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[3]UniDistance Suisse

ABSTRACT

In this talk, a model reduction approach for linear time-invariant second order systems based on positive real balanced truncation is introduced. The method guarantees to preserve asymptotic stability and passivity of the reduced order model as well as the positive definiteness of the mass and stiffness matrices. Moreover, an a priori gap metric error bound is obtained. Besides the theoretical foundations, the numerical challenges will be discussed. The presentation will be concluded by numerical examples illustrating the approach.

Data-driven methods for modeling complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEEP GENERATIVE MODELING FOR DATA-DRIVEN IDENTIFICATION OF NOISY, NON-STATIONARY DYNAMICAL SYSTEMS

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ABSTRACT

An important challenge in many fields of science and engineering is making sense of a deluge of time-dependent measurement data by recovering the governing equations in the form of ordinary or partial differential equations. We are interested in finding interpretable, parsimonious models in the form of closed form differential equations for nonlinear, noisy, and non-stationary dynamical systems. To this end, we propose a machine learning method that performs system identification in such systems.

An array of methods so far have addressed noisy and limited data; however, the problem of non-stationarity, when parameters describing the differential equations have explicit time dependence, has received considerably less attention. In this work, we combine a framework for data-driven discovery of stochastic differential equations using hypernetworks and the SINDy (sparse identification of nonlinear dynamics) method with a separate neural network module that identifies switches in the parametric time dependencies. The result is a novel approach – dynamic HyperSINDy – to system identification of stochastic, non-stationary dynamical systems. We test our method on synthetic data using simple canonical systems, including non-linear oscillators with underlying time-dependent parameters, and the chaotic Lorenz system. The aim is to extend dynamic HyperSINDy to a wide range of problems, specifically on dynamic systems where complex parametric time dependencies are expected.

Advances and applications of polytopal methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADAPTIVE PHASE FIELD MODELING OF HYDROGEN ASSISTED CRACKING USING SCALED BOUNDARY FINITE ELEMENT METHOD

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ABSTRACT

Hydrogen-assisted cracking (HAC) poses a significant threat to the structural integrity of materials, particularly in industries such as petrochemical, aerospace, and energy. The interaction of hydrogen with metals, facilitated by chemical reactions, corrosion processes, or exposure to hydrogen-containing environments, is a crucial factor influencing crack growth.

The relatively small size of hydrogen atoms allows for absorption and diffusion into the metal lattice, accumulating in stress concentration areas and grain boundaries. This accumulation weakens atomic bonds, locally increasing brittleness and causing premature metal failure. Predicting and understanding these catastrophic failures is essential, and existing models, such as those in Finite Element Method (FEM), often face limitations due to the need for highly refined meshes.

This study aims to effectively predict hydrogen-assisted cracking using the Scaled Boundary Finite Element Method (SBFEM) and an adaptive Phase Field Model (PFM). The adaptive quadtree mesh provides computationally faster solutions, with the expense of hanging nodes.

SBFEM, unlike conventional models like FEM, Boundary Element Method (BEM), or eXtended Finite Element Method (XFEM), efficiently handles hanging nodes, making it suitable for polygonal structures. The phase field model is employed for damage prediction, capable of forecasting all stages of crack development, including initiation, propagation, and failure.

In this work, a staggered approach is used to solve elasticity, phase field, and diffusion equations. The elasticity equation is two-way coupled with the phase field equation, as the phase field value influences material stiffness, and strain energy affects the phase field variable. The diffusion equation is one-way coupled to both elasticity and phase field equations, capturing the impact of hydraulic stress on hydrogen concentration and its subsequent effect on the critical energy release rate, altering the phase field value.

Validation of the proposed numerical model is achieved through a single-edge notch tension test and crack growth from an existing pit corrosion. The work is extended for examining failure patterns in a hydrogen storage tank with an initial crack. Results indicate close agreement with existing models in all scenarios, affirming the effectiveness of the proposed framework in predicting hydrogen-assisted cracking.

Advanced computational mechanics based on data-driven techniques for structure, structural dynamics and aeroelasticity
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ESTIMATION OF GRINDING CONTACT STIFFNESS AND DAMPING PARAMETERS FROM DYNAMIC OUTPUT ONLY USING HUNT-CROSSLEY FORCE MODEL AND UNSCENTED KALMAN FILTER

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ABSTRACT

A new method combining the Unscented Kalman filter and the operational modal analysis is presented for estimating experimentally the stiffness and damping at the contact point of a grinding process by a flexible manipulator. The Hunt-Crossley force model is proposed for the force contact considering the flexibility of the manipulator structure and is rewritten in a state form as functions of the contact stiffness and damping. The Unscented transform is used to linearize the nonlinear measurement functions and therefore the Unscented Kalman filter can estimate and update the stiffness and damping parameters from the state model. The method is applied to a real grinding process using a flexible manipulator where only the dynamic responses are employed to estimate the contact stiffness and damping parameters. This method promises a convenient and practical technique for estimating the operational machining parameters and can be effectively used to develop a vibration control strategy in machining.

16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics

Advances in discretization techniques, element technology, mesh adaptivity, and solution strategies for inelasticity, localization, and failure

July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A COMPUTATIONALLY EFFICIENT METHOD FOR CONSIDERING A LARGE NUMBER OF NONLINEAR MULTI-POINT CONSTRAINTS WITHIN THE FINITE ELEMENT METHOD

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ABSTRACT

The modeling of nonlinear constraints plays an important role in various problems in computational solid mechanics, especially in the context of large elastic and inelastic deformations. Among other things, they can be used for the subsequent consideration of rigid inclusions in a body originally modeled as deformable, without requiring a remeshing of the considered domain and thus contributing to a rapid modeling building. Further examples are the modeling of shear force release in frame structures under large displacements and rotations, or the modeling of deformation-dependent Dirichlet boundary conditions. In the context of the finite element method, the constraints refer to the nodal degrees of freedom; if several nodes are involved, they are referred to as multi-point constraints. One method for considering constraints is master-slave elimination, which, in contrast to Lagrange multipliers and the penalty method, offers the advantage of reducing the dimension of the problem [1]. However, the existing master-slave elimination method is limited to linear constraints.

The presentation introduces a new master-slave elimination method for the treatment of arbitrary nonlinear multi-point constraints [2]. The method is based on a mathematically rigorous derivation, where an optimization problem with constraints is chosen as the starting point. It is transformed into a modified optimization problem without constraints using the implicit function theorem. In order to perform this transformation, the set of slave degrees of freedom must be chosen in such a way that the Jacobian matrix derived from the constraints fulfills several conditions. The derivation is general and is not restricted to specific constraints. As part of the algorithmic implementation, it was possible to separate the presented method itself from the definition of the individual constraints. In the context of several numerical examples, the new method is compared with the existing methods. The results show that the new method is as accurate, robust and flexible as the Lagrange multipliers and is more efficient by reducing the total number of degrees of freedom, which is particularly advantageous when a large number of constraints have to be considered.

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Certification of simulations and model adaptation in computational science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADAPTIVITY AND UNCERTAINTY OF MULTI-FIDELITY SURROGATE MODELS FOR SHAPE OPTIMIZATION

Jeroen Wackers[*1], Hayriye Pehlivan Solak[21], Riccardo Pellegrini[3], Andrea Serani[3] and Matteo Diez[3]*

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ABSTRACT

Accurate simulation-based design optimization (SDDO) of innovative vehicles requires physics-based high-fidelity simulations, such as the Reynolds-averaged Navier-Stokes (RANS) solvers, which are usually computationally expensive. Therefore, simulations are often combined with surrogate models, fitted through the results of a limited number of evaluations. Furthermore, multi-fidelity approaches [1] are used to further reduce the computational effort of the SDDO process, by combining a few accurate but expensive high-fidelity simulations with several less accurate but faster to evaluate low-fidelity ones. Finally, efficient adaptive sampling of the surrogate training set further increases the performance for multi-fidelity surrogate-based SDDO.

The paper addresses the estimation of the uncertainty associated with the surrogate model prediction, which is crucial for driving most of the adaptive sampling approaches and assessing the quality of the surrogate model, in case of training data affected by numerical noise. The key to our approach is to divide the uncertainty into separate contributions from the interpolation, the training data, and the multi-fidelity corrections.

Surrogate models and interpolation uncertainty are reconstructed with Stochastic Radial Basis Functions (SRBF), that use a range of RBF fits with different kernels [2]. In the proposed approach, the noise in the training data is reduced by reconstructing filtered data in the training points, which are then interpolated with standard SRBF. For the filtering, RBF surrogates with a number of kernels smaller than the number of training points are least-squares fitted through the data. The uncertainty due to the noise filtering is estimated as the variance of the reconstructions. Finally, for sparse datasets the prediction uncertainty is modeled as a parabolic function based on the distance to the nearest and the number of available training points.

The method is applied for analytical test problems and the optimization of a lifting hydrofoil, addressing its efficiency. Numerical simulations are performed with the flow solver ISIS-CFD and fidelity levels are obtained with adaptive grid refinement.

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Recent advances in computational fracture mechanics and failure analysis
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EVALUATION OF CRACK PROPAGATION CRITERION USING LOCAL APPROACH UNDER EXTREMELY LOW CYCLE FATIGUE

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ABSTRACT

It is important for piping to predict unstable failure in a structure due to excessive cyclic load caused by a huge earthquake. The J-integral is used as a fracture mechanics parameter which is applicable to elastic-plastic deformation. However, J-integral cannot be effective under cyclic loading. Fatigue crack growth rate in the low cycle fatigue is evaluated by Δ J which is defined by the stress and strain ranges in a given cycle. The applicability of ΔJ has not been well verified yet under extremely low cycle loading. A generation phase analysis requires several parameters by experiment during fracture of a compact tension (CT) specimen in the previous study. Crack length and its front are the most important for load and load line displacement evaluation as a local approach. In this study, we evaluate crack propagation criterion, which has been proposed by us, with different crack propagation manners, which are simultaneous propagation of crack front, individual propagation by nodal release on a crack front and individual propagation in the mid-part of specimen under plane strain. The FE models with 1.5 and 2 inch thicknesses are 1/4 of actual CT specimen. Load control is used in experiments, however, displacement control is performed in the generation phase analysis. The approximation curve, which is determined by the experiment and represents the relationship of crack length and load line displacement, is for determinations of nodal release as crack propagation. In the ΔJ evaluation, the best result, which is the lowest deviation from the experiment, is obtained by generation phase analysis.
Critical CTOD can be corrected by stress triaxiality under the monotonic loading [1]. Additionally, stress triaxiality and equivalent plastic strain are reciprocal relations in the cracked pipe fracture [2]. The relationship between stress triaxiality and incremental equivalent plastic strain along a crack front are well examined. The incremental equivalent plastic strain exhibits some critical condition of fracture. As a result of an evaluation, the crack propagation condition is defined by equivalent plastic strain and stress triaxiality as a local approach manner. The effectiveness and applicability of three-parameter approach will be discussed in detail.

Advances in multi-scale, multi-material, and multi-component Topology Optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE DESIGN OF COATED STRUCTURES WITH SPATIALLY ROTATING LATTICE INFILL

Eddie Wadbro[*12] and Bin Niu*[3]

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[2]*Umeå University*
[3]*Dalian University of Technology*

ABSTRACT

This presentation concerns the multiscale topological design of coated structures with spatially rotating lattices as the infill. The lattice comprises a uniform microstructure that is allowed to rotate with respect to the macroscale. The spatially rotating microstructures allow the variation of lattice at the different load-carrying components, which enhances the design freedom. We optimize three key aspects: (1) the design of the structure at the macroscale, (2) the design of a microscope unit cell, and (3) a rotation field that determines, for each point on the macroscale, the relationship (the angle of a rigid rotation) between the microscale and macroscale coordinate systems. A morphology-mimicking nonlinear filtering procedure provides size control at the macroscale and microscale, while a filtering procedure utilizing an elliptic PDE ensures a smoothly varying rotation field. Numerical examples demonstrate the effectiveness and highlight some particular features of the present method with spatially varying rotation of the microstructure.

Machine learning algorithms for accelerating material characterization, discovery, design, and manufacturing processes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

REDUCED-ORDER DYNAMICS MODELING FOR ADDITIVE MANUFACTURING VIA A PRE-TRAINED TRANSFORMER NETWORK

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[1]Northwestern University

ABSTRACT

Metal Additive Manufacturing (MAM), popular in sectors ranging from aerospace to medicine, excels in creating intricate geometries, merging multiple parts into a single unit, and minimizing material waste. MAM processes typically employ complex thermal and computational fluid dynamics (CFD) models for simulation, which are time-intensive, sometimes taking days or weeks for a single high-fidelity laser track simulation. To address these computational challenges, surrogate modeling has proven crucial for enhancing the predictive and optimization capacities in manufacturing. In this work, we present a novel model hyper-reduction technique that merges the Koopman operator with an autoencoder-decoder framework while including control signal dependencies. After learning the relevant encoding, this approach leverages a transformer neural network trained on detailed physics simulations using dynamic control signals (such as laser power and scan path). This enhancement improves the model's ability to predict and flexibly adapt to changes in controlled dynamical systems, making it highly suitable for additive manufacturing process modeling. Our approach has been validated on various complex systems, including the Lorenz system with varying parameters and multi-fluid lock exchange flow under varying gravitational conditions. A critical application of this methodology has been in simulating thermal transfer in MAM processes. By treating laser path history, laser power, and laser speed as control signals of the system, we have achieved accurate predictions for MAM processes with complex laser pathways and varying laser parameters. Our results indicate that the combined use of the transformer and the Koopman operator-based approach significantly outperforms traditional models that rely solely on linear dynamics. This method demonstrates superior predictive abilities over extended periods with considerably reduced error accumulation, especially in scenarios involving control signals. This advancement marks a step forward in predictive modeling for additive manufacturing, offering a more efficient and accurate alternative to traditional simulation methods.

Emerging topology and shape optimization techniques in computational design of materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION OF CROSS-SECTIONAL PROPERTIES CONSIDERING TORSIONAL AND WARPING BEHAVIOR

Christos Kostopoulos[1], Ameer Marzok[1] and Haim Waisman[1]*

[1]Columbia University

ABSTRACT

This talk introduces a novel efficient topology optimization methodology for beams' torsion using the warping function formulation. The finite element method is used to discretize the cross-section of the beam and an efficient gradient-based optimization problem is formulated to optimize the relevant parameters corresponding to the torsion and warping constants of the beam. As a result, for the first time, one can optimize a beam for problems where the warping behavior is dominant. Density-based optimization is defined where the SIMP approach is utilized to penalize intermediate element densities.

A key challenge of the optimization that arises in the warping function framework is the so-called, updating right-hand side problem. That is, the forcing vector varies during the optimization as it depends on the cross-section boundaries, which are functions of the updating topology. To this end, an efficient differentiable boundary recognition algorithm is proposed. The methodology is applied to design beam cross-sections in which both torsion and warping constants are of interest. While intuitive topologies are obtained in the case of optimized torsion constant, this is not the case for the warping constant. The latter shows unique material distributions and a special dependence on the allowable material density.

Causal discovery and graphical causal models
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NEW PARAMETRIZATION OF DIRECTED ACYCLIC GRAPHS AND CAUSAL MARKOV KERNELS FOR SCIENTIFIC FEATURE DISCOVERY

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ABSTRACT

Due to the complexity of multimodal scientific datasets, causal feature detection in these datasets necessitates unsupervised representation learning methods. Physics-informed multimodal autoencoders (PIMA) have recently demonstrated successful unsupervised feature detection with variational autoencoders (VAEs) where multiple scientific modalities and physics constraints act as surrogates for the supervision labels typically needed for successful VAEs. Building upon the successes of PIMA, we present a VAE framework coupled with a trainable directed acyclic graph (DAG) to discover features with plausible causal relationships in multimodal scientific datasets. In particular, we introduce a new parametrization for learning both the edges of a DAG and the causal Markov kernels of the joint distribution of its nodes. We use this parametrization to simultaneously learn a DAG in conjunction with a latent space of a VAE. Our DAG and VAE training is performed in an end-to-end differentiable framework via a single, tractable evidence lower bound (ELBO) loss function. We achieve a single ELBO by placing a Gaussian mixture prior on the latent space and identifying each of the Gaussians with an outcome of the joint distribution of the DAG nodes. We demonstrate the efficacy of our DAG parametrization, and we test our joint VAE and DAG framework on both a synthetic and a scientific dataset. Our results demonstrate the capability of learning a DAG on discovered key features in an exploratory scientific setting.

Computational modeling of extreme-loading events
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPLORING MOMENTUM ENHANCEMENT IN EULERIAN AND LAGRANGIAN COMPUTATIONS OF HYPERVELOCITY IMPACT INCLUDING THE DART-DIMORPHOS IMPACT

James Walker[1], Sidney Chocron[1], Stephen Beissel[1], Christopher Sorini[1], Donald Grosch[1], Daniel Durda[1] and Simone Marhci[1]*

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ABSTRACT

The recent DART spacecraft impact into the asteroid moonlet Dimorphos demonstrated the phenomenon referred to as momentum enhancement (Ref. 1). The phenomenon is that in hypervelocity impact a large amount of material is liberated from the impacted body, hence providing more momentum transfer to the impacted body than just from the impactor itself. Over the years it is proven quite difficult to model this effect. The liberated ejecta material is in motion, moving in the opposite direction to the incoming impactor, and the ejecta has speeds that range orders of magnitude. Not only is it necessary through the modeling to correctly determine how much of the material is liberated from the impacted body, but also its speed at time of liberation. The crater left in the impacted body has a volume corresponding to liberated material as well as displaced (but still attached) material in the impacted body. The challenges in modeling are clarified by experiments that show various behaviors in such impacts. Experiments have been performed in speeds ranging from 2 to 6 km/s (the DART impact was a 6.14 km/s) with a variety of impacted materials and show interesting impactor-size-dependent behavior in both the amount of ejecta material (normalized by impactor mass) and momentum enhancement (normalized by impactor momentum, referred to as β, Refs. 2, 3). Computations have been performed with the Eulerian hydrocode CTH and the Lagrangian impact code EPIC. Sophisticated material models were placed in these codes to model the metal and rock materials. The results of the two different computational approaches will be compared with themselves and with experiments. Subsequent experiments have been per-formed with crushed basalt targets to try to simulate the asteroid surface impacted by DART. Computations will also be compared to these experiments. It is important to understand the mechanisms in these computations and how they contribute to the observed effects for there to be reasonable confidence in extrapolating the DART results to other asteroid impact situations.

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Advances in computational biomechanics and mechanobiology
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MIXED-DIMENSIONAL MULTIPHASE MODEL FOR COUPLING AIR FLOW, BLOOD FLOW AND GAS EXCHANGE IN HUMAN LUNGS

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ABSTRACT

Despite the clear benefits of mechanical ventilation, it can also cause ventilator-induced lung injury, especially for critically ill patients suffering from Acute Lung Injury/ARDS. The main obstacles to more protective and individualized ventilation strategies are still insufficient knowledge and understanding of complex lung mechanics in healthy and diseased states, mainly due to the limited ability for in vivo measurement and imaging on the most relevant alveolar level. Even the most powerful computational approaches, however, only focus on investigating the effect of ventilation on air distribution, tissue strains/stresses, while coupling to the pulmonary circulation is mostly neglected. This is even though the lungs' main function, namely gas exchange, occurs through a dense network of pulmonary blood vessels in the alveolar walls. Hence, the coupling between respiratory system and pulmonary circulation is crucial for getting more insight into the main purpose of ventilation: adequate oxygen supply and carbon dioxide release while keeping the tissue in a healthy state.

This contribution presents a physics-based, coupled, multi-dimensional, and multiphase poroelastic approach to computationally model airflow, blood flow, and gas exchange in human lungs. Motivated by the structure of the lungs, larger airways, and blood vessels are modeled as discrete 0D networks that are embedded into a 3D, three-phase (air, blood, and tissue) porous medium, representing the smaller airways, smaller blood vessels and lung tissue in a homogenized manner. Further, the respiratory gases, oxygen, and carbon dioxide are modeled as chemical subcomponents of air and blood with a suitable exchange model in the porous domain. To connect the homogenized and the discrete representations of airways and blood vessels, respectively, a 0D-3D coupling method is used, which allows a non-matching spatial discretization of both domains. The method couples fluid flow and species transport in these phases via an outflow condition from the tips of the discrete networks into the 3D porous medium and vice versa.

Such a comprehensive approach allows us to study the complex interplay of tissue deformation and perfusion and its effects on oxygenation and carbon dioxide release. Further, the underlying multiphase model can easily be extended to include additional phases to study pathological conditions such as water accumulation in pulmonary edema in future model stages.

Keywords: Respiratory system, Multi-dimensional modeling, Multiphase poroelasticity

Numerical modeling of granular and multiphase flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEM-LBM COUPLING: A MICRO-SCALE APPROACH FOR UNDERSTANDING UNSATURATED SOIL BEHAVIOR

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ABSTRACT

The paper investigates a major challenge in the modeling of multiphase flow in unsaturated soils where the solid skeleton deforms as water and air occupy the pore space in various proportions. One can distinguish four water saturation regimes in soil: (1) pendular state where particles are cohesively held by liquid bridges, (2) funicular state where the liquid engulfs only a few particles with air largely occupying the remaining void space, (3) capillary state where liquid with some air occlusions invades the entire void space, and (4) the fully saturated condition with liquid exclusively in the void space.
While the pendular regime is well understood, the funicular and capillary regimes require further analysis. Existing models primarily focus on the pendular regime, leaving a gap in understanding the complexities of funicular regimes due to challenging geometries of water clusters and air [1]. Thus, there is a need for a novel approach to cover transitions across all capillary regimes.

To address these challenges, this study proposes a numerical model coupling the Lattice Boltzmann Method (LBM) and the Discrete Element Method (DEM). The LBM simulates capillary bridge dynamics, solving Navier-Stokes and Allen-Cahn equations for multiphase flow in intricate pore geometries. Meanwhile, DEM, based on an elastic-plastic contact law, handles the kinematics of spherical grains [2]. This coupled approach successfully captures features such as water retention as well as mean capillary stress evolution during wetting and drying processes. The mean capillary stress, equivalent to capillary (apparent) cohesion, is calculated by subtracting grain-to-grain contact stress from the total stress applied to a granular assembly. The numerical simulations involve an initial assembly of spherical particles subjected to drying and wetting processes. A hysteresis is observed in the mean capillary stress and suction, showing the model's potential in predicting unsaturated soil behavior across various saturation regimes.

In conclusion, the proposed coupled DEM-LBM model is a promising tool for understanding unsaturated soils at the micro-scale, considering all saturation regimes, especially when upscaling the results to examine the stability of geostructures (dikes) under changing environmental conditions.

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Uncertainty quantification and reliability analysis in engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DIRECT FINITE ELEMENT TECHNIQUE FOR UNCERTAINTY QUANTIFICATION FOR STOKES FLOWS

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ABSTRACT

In the experimentation of microfluidic devices, uncertainties arising from human operation or environmental conditions often lead to discrepancies between the expected and actual velocity and pressure fields within the system. Uncertainty analysis becomes a crucial research focus in the design of microfluidic devices to predict field information and control device quality. the research work in presentation successfully developed a direct finite element analysis technique applicable to incompressible Newtonian fluids. The technique accurately evaluates extreme velocity and pressure field responses in uncertain Stokes flow under random boundary stimulus conditions. This innovative analysis technique seamlessly integrates the computational principles of traditional Galerkin finite element method with the continuum mechanics theory of load-response correlation. With the aid of mesh element model information, it efficiently predicts the extreme motion behaviors of fluids under uncertain conditions through an analytical approach.

Using a microfluidic cell culture chamber as an example, this study applies the newly proposed direct analysis technique for demonstration. To highlight the high accuracy of the predictive technology, the results are compared with numerous repeated simulations using traditional finite element methods under randomly configured stimulus conditions. The findings indicate our ability to directly and accurately analyze the statistical characteristics of uncertain flow velocity in the cell culture chamber under stochastic external pressure stimuli. This includes the average value, standard deviation, and correlation coefficient between random external pressure and the target flow velocity variable. The extreme value response of the target flow velocity is also obtained. Through multiple repeated simulations and the direct analytical approach in this study, the results show less than four-thousandths of a discrepancy. By employing this innovative mechanics theory and corresponding analytical technique, substantial savings in experimental resources and computational costs required for uncertainty analysis can be achieved. Therefore, this breakthrough significantly opens a door for overcoming limitations in the analysis and design of systems with stochastic conditions.

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Computational fluid dynamics (CFD) and fluid-structure interaction (CFSI): Methods and Applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ENERGETICS OF FLEXIBLE CHANNEL FLOW

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ABSTRACT

There are many flexible vessels in human body, such as artery, air way and urethra. When these vessels subject to a negative transmural pressure (internal minus external) while conveying flow, self-excited oscillations can occur. We explore the mechanism of self-excited oscillations in a two-dimensional rigid channel conveying laminar high-Reynolds number flow. One segment of the upper rigid wall is replaced by a flexible wall under external pressure. In particular, we construct a general framework for analyzing the energy budget of self-excited oscillations about a non-uniform basic state. We then apply this general framework to consider two particular models for the flexible wall, namely a fluid-beam model [1] and simple fluid-membrane model [2] with an external pressure gradient.

For fluid-beam model, a modified constitutive law is used to ensure the elastic beam is energetically conservative. We solve both the steady and unsteady systems using finite element method with adaptive mesh. The steady system shown multiple steady configurations: an (inflated) upper branch and a (collapsed) lower branch, connected by a pair of limit point bifurcations to an unstable intermediate branch. Both upper and lower steady branches can each become unstable to self-excited oscillations. In addition, detailed energy budget over a period of oscillation was calculated, where we shown that both upper and lower branch instabilities require an increase in the work done by the upstream pressure to overcome the increased dissipation.

For fluid-membrane model, numerical simulations indicate that the baseline state (with Poiseuille flow and a flat wall) exhibits two unstable normal modes: the Tollmien–Schlichting (TS) mode and a surface-based mode which manifests as one of two flow-induced surface instabilities (FISI), known as travelling wave flutter (TWF) and static divergence (SD), respectively. We find that both FISI are primarily driven by the working of normal stress on the flexible wall, lower-branch SD has negative activation energy, while upper-branch SD approaches zero activation energy in the limit of large wall damping.

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ON THE CONVERGENCE OF LUMPED MASS GALERKIN MESHFREE METHODS

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ABSTRACT

The lumped mass matrices have been widely used in Galerkin meshfree methods with explicit time stepping due to their simplicity and efficiency. However, owing to the complexity of meshfree approximants, i.e., the moving least squares or reproducing kernel shape functions, there still lacks a theoretical assessment of the accuracy of lumped mass Galerkin meshfree formulation. This work presents a rational theoretical estimate on the frequency accuracy of lumped mass Galerkin meshfree methods [1]. The proposed methodology is completely based upon the reproducing or consistency conditions of meshfree shape functions and their gradients, which successfully circumvents the fundamental difficulty associated with the use of complicated expressions of meshfree shape functions. The frequency error measures are attained for the lumped mass Galerkin meshfree formulation, which show an important odd/even basis degree discrepancy feature. More specifically, the lumped mass Galerkin meshfree formulation using a pth degree basis function yields (p+2)th order of accuracy when p is even, and (p+1)th order of accuracy in case that p is odd. In addition, it is shown that the results of lumped mass Galerkin meshfree methods are polluted by non-physical spurious modes, which on the other hand can be suppressed through replacing the conventional non-interpolatory shape functions by the interpolatory shape functions [2] in meshfree formulation. The theoretical findings are well confirmed by numerical results.
Acknowledgements: The support of this work by the National Natural Science Foundation of China (12072302, 12372201) is gratefully acknowledged.

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Modeling, optimization and computational analysis of metamaterials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NOVEL 3D TOPOLOGICAL METAMATERIAL FOR POLARIZATION-DEPENDENT MULTILAYER ELASTIC WAVE CONTROL

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ABSTRACT

The achievement of high-quality wave concentration and manipulation has always been considered as state-of-the-art technologies, especially for integrated photonics, acoustics, and mechanics. The exploration of topological phase of matter provides abundant design tools for robust waveguiding that is immune to back scattering at small defects and sharp bends. Recent research has extended the elastic wave manipulation from 2D edge waveguiding to 3D planar waveguiding. However, most of the designs are limited to single-modal and single-frequency wave propagation along the designed plane. This paper introduces a novel 3D topological metamaterial structure whose geometric parameters are intentionally configured to obtain dual-modal topological states at distinct frequencies. A comprehensive parametric study is presented to demonstrate bandgap controllability and to establish a design principle with unwanted mode prevention capabilities. Topologically protected interface modes with either large group velocity or near-zero group velocity along the z-direction are determined. Full-scale finite element simulations are employed to uncover the elastic wave propagation behaviors. The interesting layer-locked and layer-unlocked waveguiding based on excitation polarization and frequency for a straight path and a zig-zag path are demonstrated. The outcome of this work suggests abundant potential applications related to elastic wave control such as wave filters, energy harvesters, mechanical computers, etc. This work may also help inspire future research for more complex multi-modal waveguiding in 3D space.

Catastrophic failure mechanics and numerical modelling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TYPHOON IMPACTS ON OFFSHORE WIND TURBINES IN CHINA WATERS REGARDING SPATIOTEMPORAL EFFECT

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ABSTRACT

Normally, the diameter of a mature typhoon is generally more than 100km, with different areas in meteorological characteristics. During the life cycle of a typhoon, its location and structure will change significantly, leading to dramatic changes in the wind speed field of the LOWT at a fixed site. The scales and physics involved in turbine-typhoon interaction is a typical multi-scale mechanical problem, where typhoons are mesoscale phenomena while the destruction of wind turbines occurs on the microscale. Investigating the spatiotemporal typhoon impacts on the inflow wind speed field is paramount for solving this multi-scale mechanical problem. This comprehensive understanding will facilitate the identification of design ultimate loads and enable more reliable service cycle performance. The current project aims to qualitatively and quantitatively analyze the spatiotemporal typhoon impacts on offshore wind turbines in China waters for the worst-case regarding the spatiotemporal effect. This comprehensive understanding will facilitate the identification of design ultimate loads and enable more reliable service cycle performance.

The manuscript is organized as follows: Section 2 introduces the eventual worst-case scenario in China waters. The information of LOWT and offshore wind farm (OWF) is detailed in Section 3. Then, Section 4 presents an analysis framework for spatiotemporal typhoon effects on wind speed field, which is based on a data-driven typhoon wind speed field model developed and the extreme value estimation method used in data analysis. On these bases, Section 5 presents the typhoon-induced wind speed field of different LOWTs at the same time, addressing the influence of spatial impacts on the inflow wind speed field. Section 6 presents the typhoon-induced wind speed field of different times for the same LOWT, addressing the influence of temporal impacts on the inflow wind speed field. The paper ends with a discussion of spatiotemporal typhoon impacts on the inflow wind speed field for the worst-case assessment regarding offshore wind power in China waters.

Computational mechanics in Canada and China: Current states of shared scientific interests and opportunities for the future cooperation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MESH DEFORMATION METHOD BASED ON DISPLACEMENT NORMAL PROPAGATION AND DUAL QUATERNION FOR ORTHOGONALITY PRESERVATION AND HIGH EFFICIENCY

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ABSTRACT

Mesh deformation technique is commonly used in CFD simulations with moving boundaries because of its high efficiency and mesh consistency, such as unsteady flow, aeroelasticity, and aerodynamic shape optimization, whose deformed mesh quality and efficiency are of great importance. For the purpose of orthogonality preservation and deformation efficiency improvement, this paper introduces a new mesh deformation method based on displacement normal propagation and dual quaternion.

The translational and rotational motions at the boundary points are measured in a uniform way using dual quaternions. Then their total displacements are propagated to the corresponding volume points along the normal under the control of the damping function. Compared to the popular radial basis function (RBF) method[1], this method couples the displacements in all directions, preserving the orthogonality and maintains normal distribution of the near-wall mesh, preventing element inversion. And compared to the traditional quaternion method[2], it eliminates the dependence of deformation effect on rotation center selection and avoids complex interpolation.

In order to expand the application scenarios, the proposed method are combined with the RBF method into a hybrid method to cope with topologically complex mesh. The former is dedicated to dealing with the points inside the boundary layer, which always has normal correspondence whether the surface mesh is structured or unstructured. And the latter handles the points outside, whose support points are chosen from the points in the outermost layer. The pure RBF method in the whole domain needs abundant support points to guarantee the accuracy near the boundary and prevent element inversion failure, which is computationally expensive. But benefiting from valid processing of the near-wall elements, the hybrid method requires much fewer support points to ensure the mesh validity outside the boundary layer only, reducing the calculation costs and improving deformation efficiency greatly.

Two typical test cases with different mesh features and deformation modes, fluctuation deformation in fish cruise and bending deformation of a missile, are carried out to demonstrate the superiority of the proposed method in mesh quality and deformation efficiency. The influence of the damping radius and the necessity of quaternion smoothing are also discussed.

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Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE FORCE-FREQUENCY RELATIONSHIP OF THE THICKNESS-STRETCH VIBRATIONS OF QUARTZ CRYSTAL PLATES

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ABSTRACT

Quartz crystal resonators are one of the widely used sensitive elements of force sensors with increasingly broad applications, particularly in robotics. Current quartz crystal force sensors are made with AT-cut quartz crystal resonators vibrating at the thickness-shear (TSh) vibration mode, and the force-frequency relation is a typical hyperbolic curve. A thorough examination of the vibration equations of quartz crystal plates reveals that the thickness-shear vibration mode is coupled with the applied force in stresses indirectly because usually the force is exerted in the wave propagation direction and not a quantity varying along the thickness. As a result, the coupling with the thickness-shear vibration is not direct, and the effect is complicated and weak as can be seen from the hyperbolic relation between the force and frequency. To be able to obtain the frequency shift as known with the Sauerbrey equation of the quartz crystal microbalance, a new vibration mode has to be selected for possible direct coupling with the stress resultant from the applied force, and a linear relation between the stress and frequency can be obtained. A further examination of the coupled thickness-shear vibrations of an infinite quartz crystal plate shows that while the plane stresses are coupled indirectly with the thickness modes, the thickness stress perpendicular to the plate surface is directly coupled to the thickness-stretch (TSt) vibration mode. Consequently, the force-vibration relationship will be linear with the applied stress, and the sensitivity is also proportional to the ratio of stress and corresponding elastic constant. Of course, the vibration frequency will be doubled from the thickness-shear vibration mode. The vibrations of the coupled thickness-stretch mode of an AT-cut quartz crystal plate are analyzed for frequency and sensitivity to enable the design and optimization of a force sensor application. It is believed such an exploration will improve the current technology in force sensor development to satisfy increased demands for sensitive and reliable devices in fast-growing industries with intelligent features. The thickness-stretch vibration mode is not utilized in resonators for oscillators and filter applications, but it is possible to be the core element of a force sensor with the unique force-frequency relation to improve current design and deliver novel products amid the strong demands for technology development.

Fluid dynamics and SciML: Navigating challenges and seizing opportunities
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CONDITIONAL NEURAL FIELD-BASED LATENT DIFFUSION MODEL FOR STOCHASTIC GENERATION OF SPATIOTEMPORAL TURBULENCE

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ABSTRACT

Turbulent flows, characterized by their chaotic and stochastic nature, present significant challenges in predictive computational modeling. Traditional eddy-resolved numerical simulations, though detailed, require extensive computational resources, limiting their applicability in various engineering scenarios. In response, deep learning-based surrogate models have emerged, providing data-driven solutions. However, these models frequently struggle to capture the intrinsic chaotic and stochastic behaviors characteristic of turbulent dynamics, primarily due to their deterministic frameworks.

This study introduces the Conditional Neural Field-Based Latent Diffusion Model (CNF-LDM), an innovative generative framework employing probabilistic diffusion models for the versatile generation of spatiotemporal turbulence across diverse conditions. The CNF-LDM synergistically integrates a conditional neural field (CNF) encoding with a latent diffusion model, facilitating memory-efficient generation of spatiotemporal turbulence. This method also leverages Bayesian conditional sampling, enabling the unconditional model to directly accommodate a broad spectrum of conditioned turbulence generation scenarios without the need of re-training. We have rigorously evaluated CNF-LDM through a series of numerical experiments, demonstrating its versatility and efficacy in generating turbulent flows. The outcomes of these experiments highlight the transformative potential and substantial progress represented by CNF-LDM in the domain of turbulence generation. This model not only overcomes the limitations of existing deterministic deep learning approaches but also offers a more efficient and adaptable method for simulating complex turbulent phenomena.

Recent advances in meshfree and particle methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ANALYSIS OF SPH ALGORITHM FOR ELASTIC-PLASTIC LARGE DEFORMATION

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ABSTRACT

SPH (smoothed particle hydrodynamics) is a gridless Lagrangian technique that is attractive as a possible alternative to the numerical technique used to analyze large deformation events. The high-velocity impact problem is successfully simulated by introducing the strength of material into the SPH method by considering deviatoric stress and simple elastic-plastic constitutive equation. However, there are still many problems in applying the SPH method to the large deformation analysis of solid problems in relatively low-velocity impact. In the conventional SPH method, numerical fracture due to the loss of interactions among particles, which annoys the ability and the accuracy of the SPH method. Additionally, for elastic-plastic deformation of metals in low-velocity impact, the constitutive equation is essential to describe the stress state of the structure accurately. Therefore, the incremental theory of plasticity is adopted to establish the stress-strain relationship for elastic-plastic large deformations of structures in low-velocity impact.

To prevent the numerical fracture, we introduce the artificial stress and conservative smoothing method in the SPH algorithmic framework. The influence of parametric of the two methods for removing numerical fracture is analyzed. In addition, an alternative method for improving numerical fracture, the spatially adaptive particle splitting method, is suggested. The two-dimensional impact case of metal sphere on thin metallic plate is simulated by finite element and improved SPH method, and the results of such two methods are basically consistent. The validity of the improved SPH algorithmic framework has been proved and the approach achieves certain achievements in removing numerical fracture. The stress response of the plate at different impact velocities is also discussed using the improved SPH method. The result indicated that the improved SPH method removes the numerical fracture, and it avoids the influence of parameters. It is an optimal alternative compared to the artificial stress and conservative smoothing method. The conclusions obtained provide reference for the description of the large deformation behavior of elastic-plastic solid material and have great significance in further promoting the application of the SPH method in the field of solid dynamics.

Computational mechanics in high-strain rate and impact engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PARAMETER OPTIMIZATION OF MJC MODEL AND SIMULATION OF HULL BEAM STRUCTURE FRACTURE

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ABSTRACT

Due to the excellent anti blast and impact properties of Q345 high-strength steel, it is often used in key components such as deck structures of ships. The study of its dynamic material properties has practical guiding significance. This article is based on the testing results of a universal material testing machine and a separated Hopkinson compression bar system, and obtains the material properties under different strain rates, temperatures, and stress states, respectively. At the same time, a series of related experimental studies were conducted under shear conditions to analyze the fracture performance under low stress triaxiality. In order to improve the accuracy of MJC constitutive relations and fracture criteria, six parameters including temperature terms were recalibrated for the above two indicators by combining experimental measurement methods and numerical simulation results. Afterwards, in order to verify the effectiveness of parameter calibration in the MJC model, the Q345 steel Taylor rod impact rigid target plate test results based on the first stage light gas gun system were analyzed, and a numerical model of Taylor impact test was established. The MJC model has good prediction performance under low-speed conditions, but there is a significant error in the prediction of Taylor pier diameter under medium to high-speed conditions. To reduce prediction errors, in-depth analysis is conducted from multiple perspectives such as yield plateau, strain rate sensitivity coefficient, and transformation of high strain rate plastic deformation mechanism. Research has found that the yield plateau has little effect on the predicted results; Although the strain rate sensitivity coefficient effectively reduces the prediction error of cross-sectional area, it cannot accurately predict the shape characteristics of Taylor rods; Considering the high strain rate plastic deformation mechanism, the predicted results are converted, and the conversion results are closer to the experimental results. Simulate the damage effect of ship hull beams under underwater explosive explosion conditions, and compare the damage differences between the constitutive relationship obtained in this paper and the traditional constitutive relationship. To provide a theoretical basis for the comprehensive consideration of the transformation of high strain rate plastic deformation mechanisms in performance analysis under high strain rates.
Keywords: Q345 steel; Hull beams; Taylor rod; MJC model; test

Computational mechanics in high-strain rate and impact engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RESEARCH ON SIMILARITY LAW OF NONLINEAR SHOCK RESPONSE OF SHIP PLATE FRAME STRUCTURE UNDER UNDERWATER EXPLOSION

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ABSTRACT

The anti-explosion ability of ship grillage structure is an important index to evaluate the vitality of ships. Its model test is a low-cost and effective method to evaluate the vitality of ships and guide the design of ship anti impact structures. In view of the nonlinear and non-stationary process of underwater explosion damage to ship grillage, this paper breaks through the nonlinear effect of transient explosion impact that is not considered in the traditional scale model design, focuses on the one-dimensional nonlinear impact response of ship grillage structure, and carries out the characterization study of the similarity between model experiments and real ships. Considering that the vertical motion of the prototype and the model grillage structure in the model test obey the random walking model, the vertical impact response of the deck grillage is characterized as one-dimensional nonlinear non-stationary Brownian motion, which is described by Hurst index. Based on the classical similarity law, the similarity transformation relationship between the range R and the mean square deviation S is derived, and the Hurst index of the model and the prototype meets the equal relationship; Take a section of grillage structure on a real ship and conduct prototype, 1/2, 1/3, 1/4 and 1/5 one-dimensional nonlinear explosion impact scale simulation tests respectively. The numerical response results show obvious nonlinear characteristics, and the Hurst index of displacement, velocity and acceleration response of the model within the pulse width range is less than 5% compared with the prototype. According to the scale invariance of fractional Brownian motion, the similarity conversion relationship of multiple parameters (displacement, velocity, acceleration and mean square response) is obtained. With the mean square response as the characteristic parameter, the response value of the prototype is converted through this relationship, and compared with the model simulation results, the multi parameter response error under each scale ratio is less than 20%. It provides theoretical and technical support for conducting similar experiments on nonlinear response of underwater explosion shock of ships.

Coupled computational mechanics: Solutions for FSI simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTIPHYSICS MODEL OF HYPERVELOCITY IMPACT INDUCED PLASMA: SIMULATION AND EXPERIMENT

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ABSTRACT

During hypersonic collisions between materials, kinetic energy rapidly dissipates through various pathways. This process generates strong shock wave fronts and extreme thermodynamic states, not only within the solids involved but also in the surrounding gas. These states often lead to material ionization, forming a highly non-ideal plasma. The physical mechanisms of plasma formation and its source and composition are not yet fully understood and remain as open questions. We introduce a computational model of hypervelocity impact dynamics, accounting for fluid-solid interaction and predicting material ionization across all subdomains: the projectile, target, and ambient fluid. Our model combines the compressible Navier-Stokes equations with the non-ideal Saha equations. The Navier-Stokes equations are solved by employing a high-resolution finite volume method in the Eulerian reference frame. The material boundaries are tracked by solving two level-set equations. Since the subdomains share the same velocity field, spurious overlaps of materials are avoided. The Navier-Stokes equations are complemented by appropriate equations of state for each subdomain to account for their material behavior. As such, the metallic projectile is modelled using Mie-Gruneisen, the silicate target using Nobel-Abel stiffened gas, and the ambient fluid using perfect gas. We apply the model to the case of soda-lime glass shocked by a metallic projectile during a hypervelocity impact event. We carried out an experimental campaign to characterize pressure, density, temperature, and sound speed along the principal Hugoniot of soda-lime glass. The experimental data are used to calibrate the numerical model and a validation study is performed. The challenge of computing the numerical fluxes across material boundaries with significant discontinuities has been a topic of significant focus in the literature. We overcame this challenge by using the Finite Volume with Exact Riemann (FIVER) method, which has been validated for several multiphase flow applications. The plasma characteristics were computed by solving the non-ideal Saha equations along with conservation of electrical charge and nuclei, using a safeguarded root-finding algorithm. To demonstrate the developed computational model, we investigate the impact of a tantalum projectile onto a soda-lime glass target in an argon environment. The transport of energy between the materials during the impact event is measured and analyzed. Furthermore, the composition of the impact induced plasma, especially in the soda-lime glass, is investigated. Our results indicate that the alkaline metals (principally Na) in the glass account for the majority of the charged particles in the impact induced plasma, due to their low ionization potentials.

Catastrophic failure mechanics and numerical modelling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A STEPWISE PHYSICS-INFORMED NEURAL NETWORK FOR SOLVING LARGE DEFORMATION PROBLEMS OF HYPOELASTIC MATERIALS

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ABSTRACT

Physics-informed neural network (PINN) has been widely concerned for its higher computational accuracy compared with conventional neural network. The merit of PINN mainly comes from its ability to embed known physical laws or equations into data-based neural networks. However, when dealing with the rate-dependent nonlinear problems, such as elasto-plasticity with loading and unloading and hypoelastic large deformation, the conventional PINN cannot obtain satisfactory results. In this paper, a stepwise physics-informed neural network (sPINN) is proposed to solve large deformation problems of hypoelastic materials. The whole process of sPINN can be divided into a series of time steps. In each time step, the rate constitutive equation expressed by Hughes-Winget algorithm and momentum governing equation are incorporated into the loss function as physical constraints. The displacement and stress fields can be resolved by completing the training process of each time step. Three numerical examples are designed to validate the proposed method by comparing with the solutions of FEM. The results show that sPINN can accurately resolve the displacement and stress fields in path-dependent large deformation problems. Furthermore, the performance of the sPINN on small data sets are also discussed, which illustrates that sPINN is more capable of predicting the global solution on small data sets as compared with conventional artificial neural network.

Model-based simulations of structural responses under extreme conditions
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STABILIZED LAGRANGE INTERPOLATION COLLOCATION METHOD: A MESHFREE METHOD INCORPORATING THE ADVANTAGES OF FINITE ELEMENT METHOD

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ABSTRACT

Since most approximation functions in meshfree methods are rational functions which do not possess the Kronecker delta property, how to achieve exact integration and accurately impose the essential boundary conditions are two typical difficulties for meshfree methods. In this paper, a new stabilized Lagrange interpolation collocation method (SLICM) is proposed in which the Lagrange interpolation (LI) is employed for the approximation in a meshfree method. This method can satisfy the high order integration constraints which can conserves the high order consistency conditions in the integration form. This property leads to the exact integration in the subdomains and optimal convergence for the proposed method. Meanwhile, performing the integration in subdomains can also reduce the condition number of discrete matrix, which improves the stability of the algorithm. Since the Lagrange interpolation approximation has Kronecker delta property, the essential boundary conditions can be simply and exactly imposed like the finite element method, which further improves the accuracy of this method. Convergence studies present that the same convergence rate can be attained for utilizing the odd and even order LI shape functions, while the convergence rate is reduced if the odd order basis function is employed in the reproducing kernel (RK) approximation. Numerical examples validate the high accuracy and convergence as well as good stability of the presented method, which can outperform the direct collocation method and the stabilized collocation method based on RK approximation.

FACTORIZATION-BASED ONLINE VARIATIONAL INFERENCE FOR PARAMETER-STATE ESTIMATION OF PARTIALLY OBSERVABLE NONLINEAR SYSTEMS

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ABSTRACT

In many application areas such as robotics, financial prediction and computational neuroscience, the online procedure which estimates the parameters and states of a nonlinear system as the system is evolving is among the most crucial tasks. A good online inference method is expected to be efficient, robust and scalable to provide estimation rapidly, guarantee safety and handle different problems. However, estimating the states with nonlinear systems known in a fully online manner can be a difficult task in many cases. The requirement of learning the states and system parameters simultaneously online makes the procedure even more challenging. In recent years, some inference methods have been developed for online parameter-state estimation. However, many of these methods either are unreliable or scale poorly with high-dimensional problems. There exist a limited number of effective and scalable methods but they are normally computationally expensive, which makes them ill-suited for real-time tasks.

In this talk, we introduce an efficient and flexible variational inference scheme for online parameter-state estimation. Our method provides an approximate joint posterior distribution of the parameters and current states of a nonlinear system at every time step by assimilating data incrementally. At each time step, only the newly received data is processed to update the joint distribution. This keeps the computational cost for each step constant and avoids the requirement of storing historical data. Our method factorizes the variational joint posterior distribution as the product of marginal distribution of parameters and conditional distribution of current states given parameters. This enables our method to avoid assumptions of the joint posterior distribution structure, therefore providing a significantly more accurate posterior approximation. The marginal distribution over parameters can be learnt using an arbitrary representation family. Moreover, the conditional distribution of current states given known parameters can be obtained by any existing filtering approaches. The functional representation of hyper-parameters for the variational conditional distribution, can also be chosen arbitrarily. The choices of representation family of distributions, filtering approaches and functional representation of variational hyper-parameters can be made to achieve the speed or performance required by different tasks. The effectiveness of the method will be demonstrated by applications on low- and high-dimensional problems arising in various application areas.

Advanced materials: Computational analysis of properties and performance
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A GRAND-POTENTIAL BASED MULTI-PHASE-FIELD MODEL FOR SIMULATING THE EVOLUTION OF INTERMETALLIC PHASES IN CR-COATED ZRY-4 ALLOYS

Menghui Wang[*1] and Chen Lin*[1]

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ABSTRACT

Chromium (Cr)-coated zirconium alloys are considered a promising candidate material for accident-tolerant fuel (ATF) cladding in nuclear reactors due to their excellent high-temperature oxidation resistance under accident conditions [1]. However, a diffusion-induced intermetallic ZrCr2 layer would be formed at the coating/substrate interface at high temperatures, which significantly affects the microstructure and mechanical properties of the coating [2]. To quantitatively understand the effects of interdiffusion on the microstructure and mechanical properties of Cr-coated Zry-4 alloys, a novel method that incorporates successfully diffusion potential dependent-properties of bulk multicomponent phases into a grand-potential based multi-phase-field model is proposed, which captures the complex interplay among diffusion, interfacial morphology evolution, and stress variation in a high-temperature process. Results showed the variation of the simulated thickness of the Cr coating and the Cr-Zr interlayer with time was in good agreement with the experimental results. Moreover, many experimentally observed but insufficiently understood phenomena can be well explained through this numerical model. Specifically, the numerical simulations quantitatively revealed the influence of the grain size (or the number of grain boundaries), the initial thickness of the Cr coating, and the stress caused by the intermetallic ZrCr2 layer on the microstructure and mechanical properties of Cr-coated Zry-4 alloys. These numerical findings provide theoretical references for understanding the effects of interdiffusion and improving the material properties of zirconium-based alloy cladding used in nuclear power plants.

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INVERSE DESIGN TOWARD EXACT STATIC AND DYNAMIC BEHAVIORS

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ABSTRACT

We report a comprehensive roadmap for the inverse design of periodically architected materials. The primary focus is to achieve desirable linear static (i.e., elasticity tensor) and linear dynamics (i.e., dispersion relation [1]) properties with analytical precision. Both eigen-analysis-based methods and data-driven approaches will be examined. In addition, we also introduce our ongoing investigations based on recent breakthroughs in the inverse design for visco-elastic [2] and hyper-elastic [3] behaviors.

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Numerical modelling of composite materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STATIC BENDING RESPONSE OF SANDWICH COMPOSITE PLATES BY USING C0 ELEMENT BASED ON HIGHER-ORDER REFINED ZIGZAG THEORY

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ABSTRACT

This study aims at investigating static bending response of sandwich composite plates based on higher-order refined zigzag theory (HRZT). Recently, the authors developed the HRZT for static bending response of sandwich composite beams. This study is an extension of the application of HRZT to sandwich beams, which has been developed by authors recently. For plate applications, the inplane displacements are assumed to be higher-order zigzag functions, which allow this theory accurately modeling free-stress on the free surfaces and shear stress continuity at interfaces between layers.

The four-node quadrilateral element is developed to solve the displacements, deflections and stresses under linear static lateral loads. There are 9 degree-of-freedoms (DOFs) at each node, including two inplane uniform deformations, two rotations due to bending, two rotations due to zigzag, two average inplane strains and one deflection. There are totally 36 DOFs in one element, which is abbreviated as C0-4N-36. The stiffness matrix of C0-4N-36 can be derived by variational principle with introducing Lagrangian interpolation functions as the shape function to interpolate the DOFs with the element. A shear locking testing reveals a slow convergence speed of C0-4N-36 for large span-thickness ratio (thin plate).

In order to solve the shear locking phenomenon occurred in C0-4N-36, a modified element is created by adding four extra nodes, each of which is placed at the middle of the element edges. The extra nodes have the DOFs of deflection only, resulting 40 DOFs in the modified element. Thus, it is abbreviated as C0-4N-40. With extra DOFs, C0-4N-40 can effectively avoid shear locking problem for both thick plate (e.g. span-thickness ratio=5) and thin plate (span-thickness ratio=100). By considering some demonstration examples of sandwich plates with various material properties, geometric parameters and boundary conditions, the deflections, inplane displacements and stresses calculated by the present approach are compared with the 3D FEM models solved by commercial software ANSYS. It has proved that the solutions based on HRZT are reliable to linear static analysis for sandwich plates.

The main advantage of HRZT is that the calculated shear stresses along the thickness are continuous at interfaces between two adjacent layers. Both the deflections and inplane displacements solutions calculated by HRZT are much more accurate than those by Mindlin-Reissner plate theory, especially for the cases of thick sandwich plates. The formulations and results of HRZT plate developed in this study are applicable to aerospace engineering, naval engineering, civil engineering and mechanical engineering, etc.

Multiscale Theory and Modeling of Advanced Nanocomposites
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

UNDERSTANDING STRAIN HARDENING BEHAVIOR OF SEAWATER SEA-SAND ENGINEERED CEMENTITIOUS COMPOSITE (SS-ECC) WITH RECYCLED SILICA NANOPARTICLE (NSP)

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ABSTRACT

Seawater sea-sand engineered cementitious composite (SS-ECC) has emerged as an available alternative to conventional cement composites with the employment of tap water and river sand. Given this, SS-ECC exhibits significant potential in marine infrastructure applications, not only safeguarding embedded glass fiber reinforced polymer (GFRP) bars against water-induced degradation [1-3] but also addressing concerns regarding the depletion of natural resources. To enhance the tensile performance of SS-ECC and expand its practical utility, amorphous silica nanoparticles (nSP) derived from recycled GFRP powder are introduced into the cementitious matrix. The inclusion of nSP is anticipated to facilitate the formation of additional nuclei for calcium silicate hydrate (C-S-H) gels, thereby reinforcing the bond between polyvinyl alcohol (PVA) fibers and the cementitious matrix. However, the influence of nSP particle size and incorporation ratio remains uncertain, warranting comprehensive investigation encompassing both experimental and numerical approaches.
First, SS-ECC matrices are modified with nSP of varying particle sizes (a few to hundreds of micrometers) and incorporation ratios (0 to 5 wt% nSP/binder ratios). Subsequently, bench-scale experiments involving single fiber pullout tests and dog-bone tensile tests are conducted. Furthermore, molecular dynamics (MD) simulations are employed to model the interactions between nSP and the cementitious matrix, as well as between the cementitious matrix and PVA fibers. The findings obtained from this integrated approach are anticipated to shed light on the underlying chemical and mechanical mechanisms governing nSP-based SS-ECC.

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Acknowledgements

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Advances in damage & fracture modeling of multiphysics materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE TIP SOLUTION OF HYDRAULIC FRACTURE WITHIN HETEROGENEOUS DOMAIN

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ABSTRACT

Numerical methods have become one of the most important approaches for analyzing hydraulic fractures, which are common in the oil and gas production industry. Due to the nonlinear fluid-solid coupling, the tip solution of hydraulic fracture contains multiscale characteristics, resulting in various limit propagation regimes (such as viscosity- and toughness-dominated regimes) [1]. Regarding the more realistic and complex geological materials, layered heterogeneity plays a crucial role in fracture propagation. This work aims to reveal the multiscale tip asymptotics under the influence of heterogeneous interfaces between two different materials and provide some applications for modeling hydraulic fractures [2]. Firstly, the displacement and stress solutions are independently analyzed in each domain using Fourier transform, and then combined through continuous boundary conditions at the interface. Then, the integral form of the balance equation is derived, with an additional term in the kernel function that is singular at the interface. A semi-infinite hydraulic fracture is considered to investigate the multiscale tip solution, a specific space mapping and a middle variable is proposed in the solving algorithm. A remote force is defined to account for the influence of the heterogeneous interface, and its effects at the near-tip, intermediate, and far-field scales are analyzed through asymptotic analysis and validated using numerical solutions. It is indicated that the solution at the intermediate scale displays the unique characteristic of the heterogeneous domain. When the crack tip is located in front of the interface, there exists an implicit solution form that depends on the interface property at the intermediate scale instead of a matching solution for both near-tip and far-field solutions. Once the crack tip passes through the interface, an additional interface solution is integrated with interaction from the transition solution. It is pointed out that two propagation aspects of hydraulic fracture should be modified because of the asymptotic behavior, one is the failure criteria and the other is the limit propagation regime in the adjacent region of the heterogeneous interface. This work provides a fundament knowledge for hydraulic fracture in layered structures and has potential application in numerical modeling through specific tip-enhanced algorithms.

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Recent advances in partitioning method and interface mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTIPHYSICS MODELING FOR LASER ABLATION BEHAVIOR OF COMPOSITE STRUCTURE SUBJECTED TO HIGH-SPEED AIRFLOW

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ABSTRACT

When the composite structure is subjected to high-power laser irradiation and high-speed airflow, its ablation behavior presents significant localized characteristics and strong coupling effect. In this work, a coupled fluid-thermal-ablation model is developed to quantitatively investigate the localized coupling effects. Here a loosely coupled scheme with second order temporal accuracy is utilized to improve the coupling efficiency, and a high-quality mesh reconstruction method combining the Arbitrary Lagrange-Euler (ALE) algorithm and Radial Basis Function (RBF) interpolation algorithm is established to capture the moving boundary of the localized ablation pit with large deformation. The model is validated by simulating the laser ablation behavior of C/SiC composite plate subjected to the hypersonic airflow, and the predicted ablation pit profile shows a good agreement with the available experimental result. Analytical results show that as the evolution of the localized asymmetric ablation pit induces transformation of the flow regime from a closed pit flow to an open pit flow. Moreover, the flow regime transition would remarkably alter the localized flow characteristics, including the local static pressure and dynamic pressure, which in turn significantly affects the sublimation and mechanical erosion rates of C/SiC composite plate, respectively.

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Numerical modeling of granular and multiphase flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPLORING AN EMMS DRAG MODEL WITH TWO-PHASE FLUCTUATIONS

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ABSTRACT

Gas-solid fluidization is characterized by pervasive, dilute-dense two-phase flow structures, which need mesoscale drag modeling to account for their subgrid effects. The classic formulation of the energy-minimization multi-scale (EMMS) drag modeling requires a semi-empirical correlation of cluster diameter. To avoid using such a phenomenological description of mesoscale structures, in this work, we propose a two-level averaging approach: First, the mean drag in a fine-grid cell is defined as a weighted sum of the drag force in both the dilute and dense phases; Then, the second-level averaging is performed at the coarse-grid scale, where the unified EMMS drag is defined, and determined by performing a series expansion with respect to the phase-mean points of both the dilute and dense phases, respectively. The unified EMMS drag is validated with comparison to fine-grid simulation in a periodic domain and coarse-grid simulation of realistic fluidized beds, both showing fair agreement.

Advances in damage & fracture modeling of multiphysics materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL INVESTIGATION OF THE INFLUENCE OF HIGH TEMPERATURE GAS ENVIRONMENT ON OXIDATION AND MECHANICAL DEGRADATION OF THERMAL BARRIER COATINGS

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ABSTRACT

Failure process of thermal barrier coatings (TBCs) involves combined effect of hot gas and coolant. In this paper, we synthesize the analysis of conjugated heat transfer (CHT) and the modified chemo-mechanical theoretical model to clarify significant influence of high-temperature vapor and coolant on the oxidation of TBCs. Sensitivities of a number of factors to stress distributions and oxidation depth are investigated via. numerical simulation. The results show that:
(1) Computational fluid dynamics (CFD) model and modified oxidation model can describe the CHT and oxidation of TBCs under different conditions, representing a combination of CFD and finite element method (FEM) can well predict the complex corrosion by oxygen.
(2) The oxidation and failure of TBCs are jointly influenced by gas and coolant parameters. The initial oxidation rate increases exponentially with the increase of the gas temperature, velocity, total pressure, angle of attack, coolant temperature or the decrease of coolant velocity. The oxidation rate decreases rapidly at the early stage, resulting in an approximate parabolic thickening curve of the oxide. The oxidation curve is linear only when the gas temperature, velocity, angle of attack, total pressure and coolant temperature are small and the coolant velocity is large.
(3) During heat preserving, the out-of-plane stresses show tensile relief and compressive enhancement with the increase of gas temperature, velocity, attack angle, total pressure, coolant temperature or the decrease of coolant velocity. However, the volume fraction of oxygen has little effect on the stresses. The peak of thermally grown oxidation/bond coat (TGO/BC) interface and the valley of top coat/thermally grown oxidation (TC/TGO) interface are the locations prone to initiate cracks, and the final residual stresses at these positions after cooling also increase with the increase of the fluid parameters other than the coolant velocity, which is different from the effect of temperature holding stage. It is also noteworthy that when gas temperature is high up to 1773K or coolant velocity is lower than 50m/s, the residual stress near the peaks of TGO/BC interface decreases rapidly.
(4) The coatings can be designed by accounting for the critical stress and critical TGO thickness conditions. The design diagrams are conceived according to the numerical results, showing that increasing the Young's modulus of the TC layer and reducing the roughness of the upper surface of the BC layer according to the design curve in the diagrams is able to alleviate the stress concentration and improve the durability of TBCs.

Physical models and reduced order models augmentation with data for physics-informed machine learning in real-world applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICS-INFORMED MACHINE LEARNING FOR SOLVING THE TIME-DEPENDENT 2D COMPRESSIBLE NAVIER-STOKES EQUATIONS IN THE EVOLUTION OF THE PROTOPLANETARY DISKS

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ABSTRACT

1. Problem
Our study investigates physics-informed machine learning (PIML) for solving the time-dependent 2D compressible Navier-Stokes equations in astronomy. Specifically, the evolution of rotating accretion flows within protoplanetary disks. Gravitational perturbations from planets introduce sharp, time-dependent spatial features, complicating the solution. We aim to approximate these problems using PIML, training neural networks on physical laws without labeled numerical data.
2. Contribution
Deriving numerical solutions for these equations is notably resource-intensive. Recent strides in Machine Learning (ML) have accelerated solving these equations significantly. Nonetheless, this advancement is hampered by the ML models' heavy reliance on extensive training data. To address this, the field is shifting towards PIML, which involves training neural networks with PDEs to approximate solutions. PIML promises accurate modeling with minimal data dependency. However, it struggles with complex fluid dynamics, particularly in modeling unstable fluid flows. Our research explores the application of PIML to a complex fluid dynamic problem in an astronomical setting. Also, we introduced strategies to speed up the training process and improve accuracy.
3. Method
Our initial trials with standard Physics-Informed Neural Networks (PINNs) were unsuccessful in capturing the system's evolution, particularly the development of sharp spatial features. A detailed analysis revealed several shortcomings of the standard PINN: slow convergence, limited long-term solution fitting, cumulative deviation from physical laws, and poor performance in capturing sharp features. To overcome these, we introduced enhancements: a self-scalable activation function, an adaptive time-marching strategy with multiple networks, a biased loss function, and a spatial-temporal adaptive PDE sampling method.
4. Results
We evaluated our enhanced PIML model against traditional numerical solutions. Despite higher computational costs and increasing prediction errors over time, our model demonstrated markedly better efficiency. It achieved significantly smaller prediction errors compared to standard PINNs and successfully reproduced most spatial sharp features without requiring labeled data. This study provides a crucial reference for applying PIML to similar fluid dynamics challenges.

Constitutive modeling of complex materials with machine learning and artificial intelligence
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AUTOMATED DISCOVERY OF HYPERELASTIC MODELS FOR THE HUMAN BRAIN CORTEX THROUGH SYMBOLIC REGRESSION

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ABSTRACT

We introduce a novel data-driven framework capable of automatically identifying interpretable and physically valid hyperelastic models in terms of sparse experimental data. Leveraging symbolic regression, an evolution algorithm that explicitly generates parsimonious mathematic expressions for accurate data fitting, our approach enforces crucial hyperelasticity constraints, such as polyconvexity, to ensure physical plausibility and enhance model generalizability beyond the training data regime. Our exploration spans three distinct hyperelastic contexts: invariant-based, principal stretch-based, and normal strain-based, unveiling the versatility of symbolic regression. Validation of our methodology involves benchmark tests with synthetic data derived from five classic hyperelastic models. Subsequent application to experimental data, including three loading modes and targeting an optimal hyperelastic model for the human brain cortex, demonstrates the algorithm's efficacy. Results indicate that our symbolic regression algorithms adeptly discover accurate models with succinct mathematic expressions in invariant-based, stretch-based, and strain-based scenarios. Notably, the strain-based model exhibits superior accuracy, and all models, except for the invariant-based ones, effectively capture the inherent nonlinearity and asymmetry in human brain cortex under uniaxial tension and compression. Further polyconvexity examinations affirm the strict convexity within the training data regime and satisfactory extrapolation capabilities outside this regime for all models. However, the stretch-based and stain-based hyperelastic models might pose concerns regarding convexity violations under large deformations. Finally, robustness tests using synthetic data with noise prescriptions underscores the reliability of our proposed symbolic regression algorithms. Our study confirms the applicability and accuracy of symbolic regression in the automated discovery of hyperelatic models for the human brain cortex, highlighting promises in future applications in soft tissue modeling endeavors.

Modeling, optimization and computational analysis of metamaterials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CONTINUUM MODELLING AND ANALYSIS OF DISCRETE ELASTIC METAMATERIALS

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ABSTRACT

Elastic metamaterials are typically periodic materials possessing unit cells with engineered architecture, which make this type of metamaterials discrete in nature. Most current studies of the dynamic behaviour of these metamaterials are based on the evaluation of the property of unit cells or directly conducting analysis and simulation of the original discrete systems. Obviously, it is desirable to develop suitable continuum models capable of accurately capturing the overall dynamic property of these metamaterials. The current paper discusses the development of new two dimensional continuum models for a class of discrete elastic metamaterial systems with local rotation. For typical discrete metamaterials, the equations of motion can be obtained by making use of their geometries and material properties. In the current work, the continuum models are developed directly from the established equations of motion of the original discrete metamaterial systems. New constitutive relations are proposed, which contain new rotational degrees of freedom, in addition to traditional displacements. Evaluation of the new material properties indicates that the rotational and translational displacements are inherently coupled in this type of materials. The new continuum models are then used to study harmonic wave propagation in these materials. The resulting dispersive behaviour of the waves is discussed and compared with that from the original discrete metamaterial systems, showing an excellent agreement at least for relatively low frequencies. The general behaviour of wave propagation in the new continuous media is further studied and compared with the behaviour of traditional elastic waves. The current results show clearly the feasibility of using continuum models to describe the general dynamic behaviour of discrete elastic metamaterials.

Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CHARACTERIZING AND MODELING THE WIDE STRAIN RATE RANGE BEHAVIOR OF AIR-FILLED OPEN-CELL POLYMERIC FOAM

Xinghao Wang[*1] and Zhanli Liu*[1]

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ABSTRACT

Modeling the compression behavior of air-filled open-cell polymeric foams under large deformation across a wide strain rate range remains a challenge, as the air pressure is dominated by viscous effect or inertial effect at different strain rates. In this study, a visco-hyperelastic constitutive model is developed to describe the response of air-filled open-cell polyurethane (PU) foam under large deformation across strain rate range from quasi-static to dynamic. The time-independent response is characterized by an Ogden form strain energy potential, capturing the nonlinear behavior of the PU foam's cellular structure. For the time-dependent response, in contrast to existing studies, two time-dependent contributions are considered. The first contribution, representing the viscoelastic response of the polymer matrix, is modeled using a hereditary integral-based approach. And the second contribution from airflow resistance is quantitatively modeled through finite difference methods across a wide strain rate range. The model is validated and calibrated through experiment results. It shows that at high strain rates, the air pressure can constitute up to forty percent of the stress and thirty percent of the energy absorption contribution, while it is relatively negligible at quasi-static strain rates. Furthermore, a simplified semi-empirical formula is proposed to rapidly estimate the air pressure in open-cell foams at high strain rates. This formula demonstrates the mechanical response transition from open-cell to closed-cell foams with increasing strain rates. The study is meaningful for understanding the dynamic response and the energy absorption capabilities of gas or fluid filled open-cell foam.

Multiscale Theory and Modeling of Advanced Nanocomposites
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DIAMOND NANOTHREAD AS PROMISING 1D NANOADDITIVE: TOPOLOGY-CONTROLLED THERMOMECHANICAL PROPERTIES FOR POLYMERIC COMPOSITES

Xing-Quan Wang[*1] and Denvid Lau*[1]

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ABSTRACT

Diamond nanothread (DNT) has garnered significant interest as a carbon-based nanoadditive for polymeric materials due to its exceptional mechanical properties. DNT has been found to possess superior properties compared to other carbon additives, primarily in two aspects. Firstly, due to the strong interfacial shear force inside DNT bundle, there is no sliding problem between DNTs. This indicates that even if DNT is not well-dispersed, it will not affect the composite's performance. Since DNT is composed of sp3 carbon and lacks graphene surfaces, long-term ultrasonic treatment does not impact its performance. Therefore, more powerful treatment techniques can be used to achieve better dispersion effect on DNTs, and the mechanical dispersion technology has fewer restrictions. Secondly, the hydrogenated surface of DNT can prevent the introduction of structural defects during functionalization, resulting in a reinforced nanocomposite with superior performance. However, the exact influence of DNT in enhancing thermomechanical properties remains unclear. In this study, molecular dynamics simulation was used to identify the role of DNT with various topological structures on the glass transition temperature (Tg) of polymeric materials and to uncover the underlying mechanism of glass-rubber transition. The interaction mechanism was investigated through density functional theory, revealing the impact of DNT topological structures on the instantaneous dipole at the interface between DNT and adjacent polymer chains. Our results show that DNT with different topological structures exhibit variability in enhancing thermomechanical properties of polymeric materials, which is related to their rigidness, the dihedral angle between DNT and aromatic ring in the polymer chain, and their mechanical interlock. The transition from glass to rubber is induced by increases in intermolecular motions due to increases in free volume at the interface, which is governed by van der Waals interaction. Furthermore, we found that DNT significantly improves Tg of epoxy nanocomposite more than other carbon-based nanoadditives. These findings shed light on the thermal degradation mechanism of polymeric composite and provide guidance for improving the reinforcing efficiency of nanomaterials in engineering applications. Our research is expected to offer state-of-the-art theoretical approaches for designing new nano-additives tailored to different reinforcement needs of polymeric composite.

Quantum scientific computing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VARIATIONAL QUANTUM ALGORITHMS FOR TOPOLOGY OPTIMIZATION

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ABSTRACT

Topology optimization (TO) is the process of optimizing the distribution of materials within a spatial domain. Despite its wide scope of applications, TO is computationally expensive because of two causes. One is the large number of design variables corresponding to the design choices, and the other is the simulation that is used in evaluating the performance of each design. As the alternative computational paradigm, quantum computing can tackle the computational challenge of TO by leveraging the properties of quantum mechanics [1]. In this work, a novel variational quantum algorithm, quantum approximate Bayesian optimization algorithm (QABOA) [2,3], is developed and applied to solve TO problems. In QABOA, mixers are designed to achieve the exploration-exploitation balance for optimization. The equilibrium equations are solved with the QABOA quantum circuit consisting of phase-separating and mixer Hamiltonian operators in the alternating fashion. The rotation angles of the operations are optimized by Bayesian optimization, which is a surrogate-based global optimization scheme. The proposed variational quantum algorithms are demonstrated with truss structure optimization.

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Numerical methods, mathematical modeling and analysis in material science
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATION OF MACHINE-LEARNED INTERATOMIC POTENTIALS IN ATOMIC-SCALE SIMULATIONS AND BEYOND

Yangshuai Wang[*1] and Christoph Ortner*[1]

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ABSTRACT

This presentation will explore recent advancements in the field of machine-learned interatomic potentials (MLIPs), their impact on molecular simulations, and their potential for enhancing our understanding of materials behavior at the atomic scale and beyond. Starting with an overview of the Atomic Cluster Expansion (ACE) method, we will delve into its construction, recent advancements, and its role in molecular dynamics simulations. We will then discuss the generalization error analysis of ACE for simulating crystalline defects, focusing on defect equilibrium studies. Furthermore, we will explore various applications of MLIPs in materials science at the atomic scale. Finally, we will introduce MLIPs-assisted coarse-grained molecular dynamics, a method that extends simulation scales in both temporal and spatial domains using the state-of-the-art ACE method.

Machine learning and multiscale modeling for complex materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ACCELERATING MATERIALS DESIGN VIA COMPUTATION AND MACHINE LEARNING COMBINED APPROACHES

Yanming Wang[*1]*

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ABSTRACT

A long-standing challenge for materials design is to clarify materials microscopic features, and discover their linkage to macroscopic properties and processing parameters. With the recent development of computing equipment and algorithms, modeling and simulations, assisted by artificial intelligence techniques, have become a promising means to tackle the above problem. In this presentation, computation-based strategies for accelerating materials design will be discussed, through the demonstration of three examples from different aspects on combining modeling and machine learning. In the first example, an effective ensemble learning framework was proposed, for automated identification on atomic crystal structures from molecular dynamics trajectories, as a generalizable tool to extract materials descriptors. In the second example, Bayesian optimization guided coarse-grained molecular dynamics simulations were performed, to systematically investigate the effects of molecular level material properties on lithium-ion transport in polymeric material systems, for promoting an efficient screening of solid polymer electrolytes. In the last example, a three-dimensional generative-adversarial-networks-based model was established, as an attempt toward inverse design of composite materials with complex structures and multiple optimization objectives.

Advances in numerical methods for solution of PDEs
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

UNVEILING A NOVEL FLUID-STRUCTURE INTERACTION MODEL AND 3D HEXAGONAL CHANNEL NETWORK FOR ARTIFICIAL PANCREAS OPTIMIZATION

Yifan Wang[*1] and Suncica Canic[2]*

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ABSTRACT

An artificial pancreas is a medical device designed to mimic the functions of the natural pancreas, which is responsible for regulating blood sugar by producing and releasing insulin. The significance of this endeavor is underscored by the potential to revolutionize diabetes treatment. Inspired by the artificial pancreas design from our collaborator at UCSF, which involves a bioartificial organ scaffold architecture encapsulating insulin-producing cells, we embarked on developing a fluid-structure interaction model to comprehensively analyze the flow dynamics within the device, which directly influences the effectiveness of oxygen and nutrient transport crucial for optimal device performance. To capture the intricacies of this system, we employed the incompressible Navier-Stokes equations to model blood flow through the device. Simultaneously, the elasticity of the cell scaffold was described using the Biot equation. The coupling of these two problems took place at the fluid-structure interface, highlighting the intrinsic connection between fluid dynamics and structural behavior within the device. Addressing this coupled system, we introduced a decoupling approach based on Niche's scheme, followed by a solution utilizing the finite element method. Our primary focus is on presenting a novel 3D hexagonal channel network, derived from insights gained in our previous 2D study, which demonstrates remarkable superiority in design. In this presentation, we will delve into the details of our model and numerical approach, emphasizing the effectiveness of the decoupled approach. Furthermore, we will discuss the exceptional design benefits achieved through the implementation of the 3D hexagonal geometry for the artificial pancreas device.

Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INTEGRATED MODELING OF PROCESS-MICROSTRUCTURE-PROPERTY RELATIONS IN WIRE ARC ADDITIVE MANUFACTURING

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ABSTRACT

In order to study the anisotropic mechanical properties of materials in wire arc additive manufacturing (WAAM), the temperature field during the wire arc additive manufacturing process is simulated using a double ellipsoid heat source model in this paper. A Monte Carlo model is established to simulate the microstructural changes in additive layer. The modified dislocation dynamics model is used to reveal the anisotropic mechanical behavior based on grain morphology of additive manufactured Ti-6Al-4V. The obtained results are consistent with experimental data. The mechanical performance of additive manufactured Ti-6Al-4V in the build height direction is significantly lower than arc scanning direction. When the ratio of grain size between the build height direction and the arc scanning direction reaches 3.51mm/0.5mm, the yield strength ratio reaches 857.6Mpa/905.1Mpa. Titanium alloys exhibit obvious material softening at temperatures above 600°C due to grain spheroidization. The yield strength is decreased with the increase of scanning speed, which is due to the decrease in average grain width of columnar grains.

High order methods for time-dependent problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DOUBLE-VARIABLES SECOND-ORDER EXPLICIT PRECISE INTEGRAL (DSEPI) AND ITS ERROR THEORY

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ABSTRACT

Abstract
In this paper, a new kind of double-variables explicit second-order precise integration method (DSEPI) is proposed. In order to obtain a stable numerical solution from the phase field equation of structural dynamics, we adjust the second order Taylor expansion of the general solution of the motion equation with two factors. The two factors are then determined by stability and energy conservation condition, as well as the absence of global stiffness matrix inversion. Thus, we obtained DSEPI. In fact, as an algorithm DSEPI uses nodal displacement and velocity as independent variables, and might be a rising competitor to the well-known central difference method (CDM). DSEPI has the same stable integration time step as CDM but provides a more precise solution inside the stable time step. From the perspective of engineering applications, DSEPI is of advantage compared with the CDM, because velocity is introduced as an independent variable, eliminating the need to assume initial velocity as required in CDM. The algorithm demonstrates enhanced coordination steps by steps. Both DESPI and CDM feature zero numerical damping within the stable time step. It is found that DSEPI deliver accurate free vibration displacement magnitude under sudden load, since energy conservation in the form of displacement and velocity is exact in the recurrence. Both theoretically and numerically, DSEPI demonstrates superior accuracy compared to CDM for harmonic load. Particularly, when the time step approaches critical values, the accuracy obtained by DESPI is much higher than that of CDM. Preliminary numerical tests show that DSEPI is a potential integration method for structural dynamics. Its suitability for practical engineering applications makes it a noteworthy consideration.

Buckling analysis and design of thin-walled structures based on novel and intelligent computational methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FORCE TRANSMISSION DESIGN METHOD OF STIFFENED THIN-WALLED STRUCTURES BASED ON A UNIFIED MODEL

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ABSTRACT

Stiffener design plays a critical role in achieving lightweight design for stiffened panels. In this study, we propose a force transmission design method of stiffened thin-walled structures, utilizing a unified modeling-analysis-optimization model. The foundation of this model is the nested spline model, where stiffeners are represented as curves on the surface of the panel. These curves are embedded into the parameter space of the surface, resulting in a nested geometric model. The design of force transmission is divided into two steps [1]. Firstly, clear force flow members (FFM) are generated based on the principal stress direction. Secondly, a nodal variable-based sizing-topology optimization is introduced to further enhance the lightweight design. To generate precise principal stress trajectories on free-form surfaces, we employ an iterative tracing technique to generate dense principal stress trajectory families and extract FFM using hierarchical clustering. The challenging task of generating high-precision principal stress trajectories is effectively addressed by the nested spline model. For the lightweight design of FFM, we propose a nodal variable-based sizing-topology method. The heights of FFM control points are designated as design variables, and we employ the Sigmoid function to penalize these variables and steadily eliminate pseudo-heights. Additionally, we propose an isogeometric analysis method for stiffened thin-walled structures based on nested spline models to achieve integration of modeling and analysis [2]. The nested spline model is used simultaneously in the modeling-analysis-optimization process, ensuring a unified model throughout the entire design process and avoiding the need for model conversion. We demonstrate the effectiveness and robustness of the proposed method through various benchmarks and examples with industrial backgrounds. The present design framework exhibits significant potential for application in the lightweight design of stiffened panels.

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Modeling and simulation of dynamics, stability and control of aerospace structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STRUCTURE DESIGN AND MECHANICAL PROPERTIES ANALYSIS OF MULTI-FUNCTIONAL OPERATION PLATFORM

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ABSTRACT

Aerial work platform is an important mechanical equipment for aerial work. It is an indispensable tool in the fields of high-rise building maintenance, fire rescue work, power maintenance and installation, which greatly improves the timeliness and safety of high-rise building maintenance and fire protection work. Based on the structural characteristics of the telescopic arm type working platform and the scissor type working platform, this paper designs a spider type curved arm aerial working platform. Through the analysis of the mechanical characteristics of the working platform, combined with the force of the structure when the position of the curved arm changes, the integrated design of the curved arm boom system and the wheeled outrigger chassis structure is carried out. Through the finite element simulation technology, the reliable design of the spider-shaped curved arm aerial working platform is realized. The results show that the curved arm boom system can realize multi-point operation such as rotation, expansion and vertical lifting, and has the advantages of wide operation range, high operation efficiency and small retractable space. At the same time, the wheeled chassis with legs improves the mobility and stability of the operation platform. It has important application value in new working environments such as forest farms, stations and docks.

Advanced techniques for transport phenomena in heterogenous porous media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INVESTIGATION ON THE COMBINED EFFECTS OF POROUS MEDIA DISORDER AND POROSITY ON PERMEABILITY USING THE LATTICE BOTLZMANN METHOD

Zhongzheng Wang[1], Jiachen Zhao[1], Yixiang Gan[2], Jean-Michel Pereira[3] and Emilie Sauret[1]*

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ABSTRACT

Accurate permeability prediction in porous media flow is crucial in geotechnical engineering and material science, with applications spanning the oil and gas industry, hydrology, and hydrogen fuel cells. However, conventional laws such as the Kozeny–Carman equation do not capture the influence of pore structure disorder on permeability. In this study, we numerically investigate the permeability in porous media under varying degrees of pore structure disorders and porosity using the lattice Boltzmann method. Notably, our findings reveal a twofold impact of the disorder on permeability, dependent on the porosity of the media. For media with high porosity, the permeability increases with increasing disorder; whereas for media with low porosity, an increase in disorder corresponds to greater flow resistance. To provide insights into how the solid structure affects permeability, an effective tortuosity parameter that accounts for both disorder and porosity is derived. Our results demonstrate that the modified Kozeny–Carman equation successfully predicts the permeability of porous media across a wide range of disorders and porosity.

Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A SIMULATION-DRIVEN DESIGN METHOD FOR GRADED LATTICE STRUCTURES WITH COMPLEX BOUNDARY CONSTRAINTS

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ABSTRACT

Graded lattice structures (GLS) are used widely in the areas of 3D printed sensors, personalized wearable devices, robotics, energy absorption, etc., and have a prospective future in the field of personalized medical devices. The implementation of GLS-based personalized wearable medical devices necessitates a GLS design method that can effectively tackle the challenges stemming from diverse boundary surface constraints and nonlinear contact loads, due to patient-specific care needs. In this study, the proposed GLS design approach, grounded in an automatic seed generation algorithm, emerges as a prospective solution to facilitate the broad deployment of GLS-based personalized medical devices. The proposed GLS design approach is founded on the following key elements: (a) the application of PIMesh, an automatic point cloud generation algorithm, to create nonuniform seed distributions within domains of any shape; (b) subsequent generation of raw GLS based on the seed distribution; (c) the further optimization of the raw GLS geometry based on finite element analysis. As the seed distributions are customized to adhere to the specified boundary shapes of the target GLS, and the graded mechanical properties are fine-tuned via finite element analysis, the resulting GLS ensures adherence to boundary constraints and graded mechanical prerequisites. The GLS geometry optimization method, rooted in finite element analysis, adeptly manages the non-linear contact loads commonly encountered in wearable medical devices. Several demonstrations, including a 3D-printed shoe sole and an energy absorber, have been conducted. The results affirm the efficacy of the proposed GLS design and optimization method.

Recent advances in meshfree and particle methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MOVING LEAST SQUARES IMMERSED BOUNDARY METHOD FOR SPH WITH THIN-WALLED OR SLENDER STRUCTURES

Zhuolin Wang[*1], Yi Zhang[2], Zichao Jiang[1], Bohua Huang[1], Xuan Luo[1] and Qinghe Yao[1]*

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ABSTRACT

This study presents a moving least squares immersed boundary method for smoothed particle hydrodynamics (SPH), aiming to simulate thin-walled or slender structure immersed in fluid. Based on the direct forcing immersed boundary method, the proposed method improves the velocity interpolation using the moving least squares method. In comparison to traditional SPH wall boundaries (e.g., ghost particles, fixed particle method, etc.), this method eliminates the need for multiple layers of particles, making it particularly suitable for thin-walled or slender structures. The proposed method reduces oscillations and achieves higher accuracy while retaining the advantage of immersed boundary method.

Results of three-dimensional numerical tests are presented, including impulsively started plate, flow past a cylinder, and flow past a sphere, comparing to results of other commonly used immersed boundary schemes. Compared to the diffusive direct forcing immersed boundary method, the proposed method shows more accurate lift and drag coefficients, effectively avoids mutual interference on both side of the boundary. In comparison to the direct forcing immersed boundary method using linear interpolation, the proposed method sustains more accurate computational results while effectively decreasing pressure oscillations. Furthermore, the proposed method is applied in flexible fibers fluid-structure-interaction (FSI) problems, successfully simulating the shape and movement of flexible fibers with different stiffness in three-dimensional shear flow.

Multi-scale, multi-rate damage and fracture: Models, experiments, and simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MICROPLANE CONSTITUTIVE MODEL FOR TENSILE AND COMPRESSIVE DAMAGE IN BRITTLE POLYMERS

Sanket Vinod Wardhekar[*1], Garret Smith[1] and Kedar Kirane[1]*

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ABSTRACT

This work presents a novel adaptation of the microplane constitutive model for tensile and compressive damage in brittle polymers. The salient feature of the model is the “microplane” which is an imagined plane within the material microstructure. At each material point several microplanes of various orientations are assumed to exist and various tensile and compressive damage mechanisms are formulated in terms of stress-strain vectors acting on these microplanes. The macroscopic strain tensor is projected on these microplanes to yield several strain vectors. Through the damage laws, these yield corresponding stress vectors, which are homogenized via the principle of virtual work to obtain the macroscopic stress tensor. Four damage laws are considered at microplane level, driven by the normal, deviatoric, volumetric, and shear strains, each intended to capture specific observed damage mechanisms in the highly nonlinear tensile and compressive stress strain laws of polymers. These include tensile microcracking, shear microplasticity, micro-crack friction, and far post-peak compression hardening. The model incorporates a volumetric-deviatoric (V-D) split at the microplane level, which is necessary for materials with Poisson ratios above 0.25. The model is calibrated through experimental data and is demonstrated to reproduce the intricate damage behaviours of polymers, through relatively simple damage laws. It is also shown that while the uniaxial tensile behaviour can be reproduced with single material point analyses, a specimen level (multiple material points) model is required to capture the uniaxial compressive behaviour due to the marked localization of shear damage. The model is also compared to Mohr Coulomb and Drucker Prager plasticity models and is found to exhibit better agreement with experiments.

MICROMECHANICAL CONSTITUTIVE MULTISCALE MODELING OF RATE-DEPENDENT EFFECTS IN FERROELECTRICS: A COMPREHENSIVE APPROACH

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ABSTRACT

Ferroelectrics exhibit many interesting effects, both linear and nonlinear, which is why these materials are widely used in science and industry. Moreover, it is noteworthy that the majority of these effects, particularly those which are nonlinear, are strongly rate-dependent, rendering the modeling of these intricate materials with multiple material scales quite challenging. The rate dependence is contingent on the material scale at which these distinct effects occur, yet they are all reflected in the macroscopic material behavior. Furthermore, nonlinear effects are irreversible and are accompanied by energy dissipation, which generally leads to a temperature rise of the material. For modeling the distinctive nonlinear rate-dependent effects of ferroelectric materials, there are numerous options, including microphysical and phenomenological models.

Aspects of different rate-dependent effects, as well as mutually coupled dissipative processes in ferroelectrics, in particular ferroelectric domain switching and viscoelasticity, are investigated theoretically, based on a microphysical motivated thermo–electromechanical multiscale constitutive framework. For this purpose a hybrid micromechanical–rheological constitutive model is developed and embedded in the framework of a multiscale modeling approach [1, 2, 3]. The mathematical theory is consistent against the background of rational thermodynamics and deals with two types of internal variables. The advanced modeling approach is inter alia applied to identify novel energy harvesting cycles exploiting dissipative effects, resulting in a major electric work output.

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Innovations in machine learning-enhanced uncertainty quantification for computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ENABLING PROBABILISTIC MICROWEATHER PREDICTIONS THROUGH DEEP GENERATIVE MODELING AND OPERATOR LEARNING

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ABSTRACT

Motivated by NASA's pursuit of safe, reliable, and weather tolerant urban air mobility (UAM) solutions, this work develops a framework for rapidly and probabilistically assessing microweather conditions. The approach leverages recent advances from the deep learning field to make efficient wind predictions as a continuous function of space/time while also capturing natural random variability (e.g., wind gusts). In particular, a denoising diffusion probabilistic model [1] is trained to produce realistic samples of wind speed on the periphery of a UAM operational space to serve as boundary conditions. A deep operator network (DeepONet) [2] then learns the nonlinear operator that maps samples of winds on the boundary to the microweather wind conditions throughout an area of interest (e.g., a landing zone). The framework bypasses the need for expensive computational fluid dynamics predictions and is shown to provide accurate uncertainty quantification (UQ) that can enable reliable UAM operations.

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Uncertainty quantification and reliability analysis in engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

POLYMORPHIC UNCERTAINTY QUANTIFICATION, SENSITIVITY ANALYSIS AND BAYESIAN MODELING IN MULTISCALE AND MULTIPHYSICAL FEM MODELS

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ABSTRACT

The complexity of numerical simulations, especially in multiscale and multiphysical modeling, highlights the need for polymorphic uncertainty quantification (PUQ) methods. These are vital for a comprehensive understanding of input parameters, improving model efficiency, and contributing to the optimization of complex systems. Our presentation aims to highlight various aspects of PUQ analysis using different engineering examples based on the Finite Element Method (FEM), focusing on examples from the automotive and aircraft industries, as well as examples from soil mechanics and biomechanics.

In our workflow, we start by creating a parameterized FE model along with an essential metamodel, which is particularly important for complex models to save computational time. Uncertain parameters are modeled as either aleatoric or epistemic uncertainties based on available information. Subsequently, PUQ is derived to obtain a probability of the solution of interest or to perform reliability analysis.

Key aspects to highlight include Bayesian analysis, employed to generate a metamodel. Numerical simulations provide additional knowledge to optimize estimated parameters within the surrogate model. Furthermore, the Bayesian approach refines estimated uncertainties of input parameters. When experimental data is available, Bayesian approaches can update prior assumptions for input uncertainties, thereby improving output uncertainties.

Another focus is on Variational Sensitivity Analysis (VSA), which can analyze the local impact of input parameters and can be embedded in an efficient metamodel, a so-called Gradient Enhanced Kriging model.

Additionally, we aim to highlight the relevance of a polymorphic approach, whereby both aleatoric and epistemic uncertainties can be considered. Aleatoric uncertainty requires additional information for a probability distribution of parameters, whereas epistemic uncertainty is viewed as information with missing knowledge, addressed through a fuzzy approach.

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Advanced discretization schemes and solution strategies for computational structural dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE GEOMETRICALLY EXACT BEAM IN A QUATERNION FORMULATION WITH AN ENERGY-MOMENTUM CONSERVING INTEGRATOR

Paul Wasmer[*1] and Peter Betsch*[1]

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ABSTRACT

In various engineering domains, beam models play a pivotal role in simulating slender structures efficiently. The most important model for large deformations is the so-called geometrically exact beam also often referred to as Simo-Reissner beam. The configuration manifold of the beam model is given by special Euclidean group as it describes the position of the centerline as well as the orientation of the beam's cross-section. The partial differential equations describing the behavior of the beam is usually solved with the help of the Finite Element Method (FEM). So it becomes necessary to discretize the special orthogonal group in a finite element sense.

However, discretizing the special orthogonal group proves challenging due to its non-abelian, non-additive matrix group nature under multiplication. An intriguing alternative is the use of unit quaternions for the parametrization of the special orthogonal group. Employing a Hu-Washizu-like approach for the beam enables us to mitigate locking effects. To establish a stable time integration, our objective is to devise an energy-momentum conserving scheme. By integrating the Liven’s principle into this mixed approach, we simplify the development of an energy-momentum conserving time integration scheme.

Existing literature frequently highlights the advantages of Isogeometric Analysis (IGA) over traditional FEM using Lagrangian elements, particularly in addressing dynamic challenges. We thus apply the IGA to the Hu-Washizu-like quaternion formulation of the geometrically exact beam.

CHARACTERIZATION OF LOCAL MECHANICAL PROPERTIES OF METALLIC MICROSTRUCTURE USING INSTRUMENTED INDENTATION TEST

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ABSTRACT

Instrumented indentation test is an extension technique of hardness test, in which the load-depth relationship is measured. Based on the material test, various approaches have been proposed to estimate the stress-strain curve corresponding to a tensile test. Among them, a single indentation approach based on pile-up height of the impression[1,2] has preferable feature to characterize the heterogeneity of mechanical properties in a structure such as an additive-manufactured sample[3]. In this approach, a finite element model can be constructed based on the estimated heterogeneity. Besides, the instrumented indentation test has multiscale extensibility similar to hardness test; i.e., it can be applied to micro-scale evaluations by setting a small load. In this study, the single indentation approach based on pile-up height is applied to estimation of mechanical properties in a metallic microstructure. Here, a simple constitutive model for single crystal is defined and its material constants are determined on the basis of a correlation between experiments and simulations of instrumented indentation tests. Subsequently, the applicability and limitations are discussed.

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Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFECTS OF ROTATING CYLINDRICAL ROUGHNESS AND ITS ROTATING DIRECTION ON CROSSFLOW-VORTEX TRANSITION OF SWEPT-FLAT-PLATE BOUNDARY LAYER

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ABSTRACT

The turbulent transition on the swept wing of an aircraft is triggered by the crossflow instability near the leading edge and/or the Tollmien-Schlichting (TS) instability in the downstream [1]. Also, the crossflow instability promoted by the presence of manufacture-induced surface roughness turns the entire wing surface of existing aircrafts into turbulent. Discrete roughness elements, such as cylinders, have been adapted to the wing in order to delay the turbulent transition [2]. However, despite the advantage of being the passive control, this method has not been applied to actual aircraft due to its low robustness to flight attitude such as angle of attack, i.e., flow field in the boundary layer. Recently, Wu et al. [3] studied the effect of rotating cylindrical roughness on the TS instability of the two-dimensional boundary layer, without the crossflow instability.

In this study, we study the turbulent transition process in the downstream of the rotating cylindrical roughness in a three-dimensional boundary layer by direct numerical simulations. To this end, we employ the Falkner-Skan-Cooke similarity solution to model the swept-flat-plate boundary layer and the rotating cylindrical roughness is implemented by the immersed boundary method. We compare two adjacent cylinders rotating in either the same (co-rotating) or opposite (counter-rotating) directions by varying their height and angular velocity. The gap between the adjacent cylinders is set to the most unstable wavelength at which the crossflow instability grows most rapidly.

With zero angular velocity, a crossflow vortex emerges in the downstream, leading to the turbulent transition. The co-rotating cylinders alter the vortex generation process. Under limited conditions, this alteration of the vortex structure causes a transition delay, and we find that a faster rotation eventually promotes the transition. The threshold of delay/promote also depends on the roughness height. In the co-rotating condition, the friction coefficient is higher than in laminar flow before the transition, but the transition position is delayed. In the counter-rotating condition, the friction coefficient is similar to that of the laminar flow before the transition, but the transition position is not delayed as in the co-rotating condition. In the presentation, we will further discuss how the rotating cylinders modify the crossflow vortex structures, and how they determine the turbulent transition point.

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Computational fluid dynamics (CFD) and fluid-structure interaction (CFSI): Methods and Applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SIMULATION OF FLUID-STRUCTURE INTERACTIONS USING MULTI-VELOCITY DESCRIPTION COMBINING DISCONTINUOUS GALERKIN FINITE ELEMENT METHOD AND MATERIAL POINT

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ABSTRACT

Accurate description and determination of material interfaces are important tasks for any numerical method intended to study fluid-structure interactions. Many interface tracking and reconstruction methods have been proposed and studied for this purpose.

Here, we introduce a numerical approach for fluid-structure interactions using a multi-velocity description of the materials with the combination of Discontinuous Galerkin finite element method (DGFEM) and the material point method (MPM). In this approach, no special interface tracking method is needed. All simulated materials are described by their own velocity fields. The solid materials will be simulated by MPM while the fluid materials will be handled with DGFEM. For fluid structure interaction, at each spatial location there are two velocities values, one for the fluid and one for the solid. The solid material is represented by the Lagrangian material points, which moves with the deforming solid. The positions of these material points describe the region occupied by the solid in the computational domain, which includes information about the boundaries or interfaces between the solid and fluid. The interaction of the two materials, regardless of fluid-fluid, solid-solid or fluid-solid, is modeled as the interaction force, such as drag, in the mixed cell containing any amount of materials. In our formulation, all the materials are allowed to have their own density, velocity, energy, and stress fields. The density of a material is calculated according to its own evolution equation subjected to the continuity constraint. The stress (or pressure) evolves independently according to the constitutive relation (or equation of state) of the material.

In this presentation, we will discuss the application of multi-velocity to only fluid materials interaction, only solid materials interaction and fluid structure interaction. The algorithms needed for applying the material point method to multi-velocity calculations will be discussed. Numerical examples will be provided to show validity of the method.

Quantum scientific computing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HYBRID QUANTUM ALGORITHM FOR THE LATTICE-BOLTZMANN METHOD

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ABSTRACT

The Lattice-Boltzmann method (LBM) stands out in versatile and highly parallel fluid mechanics simulations. However, increasing computational demands with finer resolution and larger domains motivate the exploration of quantum computing potential in computational fluid dynamics applications.

The LBM can be divided into two significant algorithmic steps: collision and streaming. Quantum algorithms for the LBM using amplitude encoding techniques allow the formulation of the streaming step by a unitary evolution of the state vector. Given its inherently non-unitary nature attributed to the diffusive component, the collision step cannot be directly implemented within a quantum algorithm. Hence, a Linear Combination of Unitaries (LCU) algorithm is employed to statistically implement the linearized collision step. The collision process is successful when an ancillary qubit is measured in the ground state and fails otherwise [1].

We introduce a novel hybrid quantum algorithm for the LBM, encompassing initialization, collision, and streaming as unitary quantum operators. The zeroth and first moments of the distribution functions are computed by digital post-processing at each time step. Subsequently, a unitary evolution enables linear collision, removing the necessity for the LCU algorithm. This is achieved by incorporating the quantum measurement as part of the collision operator, resulting in a fail-safe collision operator. Finally, established algorithms implement the streaming step.
Our algorithm agrees with a digital reference implementation utilizing an analytical state vector simulator. Additionally, we assess the performance of our algorithm through noise-free sampling simulators, revealing a faster convergence rate with fewer required shots. Algorithms utilizing the LCU method often demonstrate mass loss due to under-sampling errors. In contrast, our algorithm fully conserves mass for the linearized collision operator.

The Carleman linearization approximation can incorporate non-linear effects to address the collision operator's inherent non-linearity [2].
Our framework facilitates the computation of the non-linear dependence of the collision operator by leveraging the non-linear measurement process. Consequently, we can implement the non-linear collision operator without using approximate linearization techniques.

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THE WEIRDNESS OF SOFT DEFORMABLE PARTICLES SUSPENDED IN FLOWS

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ABSTRACT

Particles suspended in fluids continue to pose a challenge in various fields of science and engineering, especially for particles in the micrometer range, due to the high complexity and cost of computational models and experimental techniques. For microparticles, the particle Reynolds numbers are usually well below one, and the local flow around the particle can be described by Stokes flow, [1]. Although surface tension results in a predominantly spherical shape for microscopic droplets and bubbles, several types of deformable microparticles are nonspherical and can be deformed by the action of the fluid flow, which significantly increases the complexity of particle tracking. Examples in this area are liquid capsules, vesicles and biological cells. In recent years, these soft particles have gained considerable importance in science, especially in the pharmaceutical field, e.g. in the targeted delivery of drugs.

In this talk, we will focus on our novel computational model for tracking the motion and deformation of a large number of micrometer-sized, soft, i.e. deformable, non-spherical particles in dilute fluid flows using Lagrangian particle tracking. In this context, we use the point-particle approach since it is a common technique for modelling a large number of microparticles and has comparatively low computational requirements. Furthermore, we assume affine deformation and creeping flow around the particle, [1].

We compare the novel approach in the limit of quasi-rigid as well as for soft deformable particles with analytical and numerical results from the literature, [2], and obtain good agreement with the references. The model is further applied to simple flows such as Couette and Poiseuille flows, here we especially focus on the tank-treading phenomenon displayed by flow-immersed soft particles. Future steps include the application to technologically relevant flows, such as in realistic human lung replicas.

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Machine learning methods for multiscale and multiphysics material modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PARAMETERIZED HYPERELASTIC MATERIAL MODELING AND MULTISCALE TOPOLOGY OPTIMIZATION WITH PHYSICS-AUGMENTED NEURAL NETWORK

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ABSTRACT

In the last decades, a vast amount of highly specialized metamaterials has been developed and, with advancing requirements in engineering applications, the trend is growing. Often comprised of complex microstructures with parametrized geometry, these materials can be tailored for each specific application. Examples include lattice-metamaterials with varying radii or fiber-reinforced elastomers where the volume fraction of the fibers might vary. Since such materials behave highly nonlinear, their mechanical description is challenging. Thus, we envision the use of physics-augmented neural networks (PANNs), circumventing the current limitations of analytically formulated multiscale material models.

In [1], we apply neural networks to formulate parametrized hyperelastic constitutive models. The models fulfill all common mechanical conditions of hyperelasticity by construction. In particular, partially input convex neural network (pICNN) architectures are applied based on feed-forward neural networks. Receiving two different sets of input arguments, pICNNs are convex in one of them, while for the other, they represent arbitrary relationships, which are not necessarily convex. In this way, the model can fulfill convexity conditions stemming from mechanical considerations without being too restrictive on the functional relationship in additional parameters, which may not necessarily be convex. Two different models are introduced, where one can represent arbitrary functional relationships in the additional parameters, while the other is monotonic in the additional parameters. As a first proof of concept, the model is calibrated to data generated with two differently parametrized analytical potentials, whereby three different pICNN architectures are investigated. In all cases, the proposed model shows excellent performance.

Furthermore, in [2], we apply hyperelastic PANN constitutive models for topology optimization (TO). Using a level-set TO approach, the applicability of hyperelastic PANN constitutive models in 2D and 3D optimization scenarios is demonstrated. The optimized designs received with the PANN constitutive model are in excellent agreement with the ones received with their ground truth counterparts. Furthermore, a parametrized PANN from [1] is applied for multiscale TO. In the optimization process, both the geometry of the macroscale and microstructural parameters are optimized, where the TO with the PANN model again shows excellent results.

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Immersed-boundary variational methods: Theory, data structures, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN IMPROVED MULTI-LEVEL HP FINITE CELL METHOD FOR EFFICIENT THERMO-VISCOPLASTIC ANALYSES

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ABSTRACT

Efficient numerical integration of the weak formulation of the governing equations plays a key role in the finite cell method [2]. The challenge is even more severe for non-linear problems relying on iterative solution schemes. Higher order interpolation spaces and the geometric and structural complexity of the analysis models usually require a significant number of quadrature points to capture the analysis domain with sufficient accuracy and to ensure an adequate convergence behavior of the analysis. A remedy to an over-excessive need of quadrature points from the established recursive bi-section approach is the use of the recently proposed non-negative moment fitting quadrature approach [1, 3] which is demonstrated in this presentation in the framework of thermo-viscoplastic analyses. Instead of the conventional cell partitioning approach [2], we use non-negative moment fitting quadrature to find a priori an optimal set of quadrature points that provides the desired properties. The performance of this novel quadrature method is tested in the framework of viscoplastic analyses with a multi-level hp refined finite cell method. We present the proposed approach for smooth and non-smooth solution fields and show an extension to a thermo-viscoplastic analysis of industry-relevant models [3].

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Multiscale modeling, analysis and numerical methods of material defect and inhomogeneities
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING GROWTH AND MECHANICAL FEEDBACK IN ELASTIC BIOLOGICAL TISSUES

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ABSTRACT

The inhomogeneity of cell proliferation, apoptosis, and myosin-dependent contraction can generate elastic stress and strain in living tissues, which may be dissipated by internal rearrangement through cell topological transition and cytoskeletal reorganization. Moreover, cells and tissues can change their sizes in response to mechanical cues. We develop a continuum model based on finite elasticity and growth theory to describe the coupled tissue growth and mechanics in the Eulerian frame. We incorporate the tissue rearrangement by introducing a tissue rearranging rate and propose energy-dissipative mechanical feedback on growth. By linearizing the model, we show that the stress follows the Maxwell-type viscoelastic relaxation. The rearrangement rate, which we call tissue fluidity, sets the stress relaxation time, and the ratio between the shear modulus and the fluidity sets the tissue viscosity. We apply the model to study the tumor spheroid growth and mechanics in the context of differential growth induced by the growth-promoting factor field undergoing a reaction-diffusion process. We investigate the key parameters in the model by fitting experimental data of tumor spheroid growth. We aim to demonstrate the roles of the tissue material properties and mechanical feedback regimes on its size and mechanics regulation.

Recent advances on interfaces dynamics modeling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HOW MATHEMATICAL AI IS TRANSFORMING BIOSCIENCES

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ABSTRACT

Mathematics underpins fundamental theories in physics such as quantum mechanics, general relativity, and quantum field theory. Nonetheless, its success in modern biology, namely cellular biology, molecular biology, chemical biology, genomics, and genetics, has been quite limited. Artificial intelligence (AI) has fundamentally changed the landscape of science, engineering, and technology in the past decade and holds a great future for discovering the rules of life. However, AI-based biological discovery encounters challenges arising from the intricate complexity, high dimensionality, nonlinearity, and multiscale biological systems. We tackle these challenges by a mathematical AI paradigm. We have introduced differential geometry, algebraic topology, and combinatorial theory to significantly enhance AI's ability to tackle biological challenges. Using our mathematical AI approaches, my team has been the top winner in D3R Grand Challenges, a worldwide annual competition series in computer-aided drug design and discovery for years. By further integrating mathematical AI with millions of genomes isolated from patients, we uncovered the mechanisms of SARS-CoV-2 evolution and accurately forecast emerging dominant SARS-CoV-2 variants.

Advanced machine learning methods for multiscale modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADVANCING MULTISCALE MODELING IN POLYCRYSTALLINE MATERIALS: A NOVEL DEEP MATERIAL NETWORK APPROACH

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ABSTRACT

This study introduces an enhanced Deep Material Network (DMN) model specifically designed to analyze and model polycrystalline materials. Our method builds on the original DMN concept by Liu et al. [1]. It incorporates the interaction-based mechanisms proposed by Noel et al. [2], significantly improving polycrystalline materials' simulation efficiency and accuracy. The core of our approach involves adapting the DMN architecture to capture the complex geometry of polycrystalline materials, allowing for a more accurate representation of the interactions among different phases and, thus, better representing their textural characteristics. Furthermore, our model includes an active learning strategy to efficiently sample diverse material properties, enhancing the dataset and the model's predictive capability and robustness. This ensures that all critical data points are comprehensively covered, effectively navigating the vast material property space. A notable feature of our model is its ability to accurately and efficiently capture the polycrystalline texture during the online prediction phase. This capability is further enhanced by integrating crystal plasticity within the DMN framework, which aligns well with direct numerical simulation (DNS) results and showcases the model's high efficiency. In summary, our enhanced DMN model marks a significant advancement in the analysis and modeling of polycrystalline materials. Combining an enhanced DMN architecture and crystal plasticity makes our model a powerful tool in multiscale modeling. It offers accuracy, efficiency, and a physically meaningful interpretation of polycrystalline materials, paving the way for applications in material design and performance optimization.

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Industrial applications of IGA
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

OPENQUAD: A SEMI-AUTOMATIC AND SCALABLE UNTRIMMING PIPELINE FOR TRIMMED NURBS

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ABSTRACT

In engineering design, one of the most daunting problems in the design-through-analysis workflow is the dealing with trimmed NURBS, which often involve problematic topological information and lead to inevitable gaps and overlaps in the geometric model. Given the dominance of the trimming technology in the CAD community, fixing such a model with a watertight representation is highly desired. While remarkable progress has been made in recent years, especially with the advancement of isogeometric analysis, there still lack a fully automatic and scalable tool to achieve this reconstruction goal. To address this issue, we present a semi-automatic and scalable untrimming pipeline based on a scalable, field-aligned meshing tool QuadriFlow. On top of it, we add support for open surfaces to deal with engineering shell structures, and we perform sophisticated patch simplification to remove undesired slender patches. As a result, we obtain a watertight multi-patch NURBS with a nice semi-regular layout. Through several challenging models from industry applications, we will show that the manual intervention is minimal (i.e., tuning only a single parameter when necessary) and the pipeline can handle large-scale models within minutes.

Multiphysics biomechanics of bio- and bio-inspired soft materials: Theory, simulation and experiments
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADVANCED FLUID-STRUCTURE INTERACTION SIMULATION OF A HUMANOID BIOREACTOR SYSTEM FOR OPTIMIZED TISSUE ENGINEERING

Yuyang Wei[1], Pierre Mouthuy[1], Sarah Waters[1] and Antoine Jerusalem[1]*

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ABSTRACT

The integration of computational mechanics in tissue engineering has opened new avenues for optimising bioreactor designs as faster and more cost-effective alternatives to traditional trial-and-error experiments. In particular, the incorporation of the biomechanical environment in tissue (re)generation models can leverage recent progress made in multiphysics computational sciences. This study presents a fluid-structure interaction (FSI) simulation of a bioreactor subjected to in vivo-like conditions. This bioreactor, which integrates a flexible scaffold within a dynamic mechanical stimulation setup, mimics the complex biomechanical environment of human tissues. Our FSI simulation framework aims at predicting the impact of the flow of culture medium on cell seeding and growth. We then compare these simulation results with the cell distributions from in vitro models to optimise the bioreactor design and operation. Our FSI approach couples our solid solver (MuPhiSim) with a fluid dynamics solver (OpenFoam) using Precice. Ultimately, the proposed simulation framework aims to identify optimal operating conditions and system properties, including scaffold geometry, material properties, and fluid dynamics parameters such as perfusion velocity, to promote cell proliferation and achieve uniform seeding distribution. A distinctive feature of this research is the validation of the FSI model against in vitro experimental data. We employ fluorescence imaging to quantify cell distribution on the scaffold and compare it with simulated shear stress and pressure distributions. This comparison between fluid dynamics within the bioreactor and cell distribution patterns will provide valuable insights into the mechanical stimuli influencing cellular activities, which are crucial for designing more effective tissue engineering bioreactors.

Keywords: Fluid-Structure Interaction, Humanoid Bioreactor, Tissue Engineering, Computational Biomechanics.

Advanced machine learning methods for multiscale modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEEP MATERIAL NETWORKS FOR UNIFIED COMPUTATIONAL MULTI-SCALE MODELING OF THE HIGHLY NON-LINEAR BEHAVIOR OF SHORT FIBER-REINFORCED POLYMERS

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ABSTRACT

In competitive industrial environments, fast development processes for products with high reliability requirements are key to success. This is achieved by virtualizing the product development process to a high degree. Designing reliability of complex systems in early phases of the product development process in the absence of physical prototypes requires the use of precise simulation methods. For components made of short fiber-reinforced polymers, accurate modeling and simulation is a non-trivial task since the manufacturing-induced microstructural configuration of the material impacts the thermo-mechanical behavior of the macroscopic component. Conventional anisotropic modeling approaches typically used for these tasks do not accurately resolve the microstructure-property relation and require a time and cost intensive material parameter identification. Numerous experiments are required with different combinations of load directions versus material orientations. The recently developed deep material networks (DMNs) [1, 2] have the potential to relieve this pain by either generating virtual data for calibrating classical anisotropic models [2] or by being used as a material model in finite element analyses on component level directly [3]. DMNs are extremely fast and accurate surrogate models for high-precision fast Fourier transformation-based simulations (FFT) on realistic 3D microstructures. In an offline phase, numerous micromechanical FFT simulations are performed to generate linear elastic training data. Once trained, the DMN is used in an online phase to inversely identify the constitutive parameters of the non-linear individual phases in the composite based on sparse experimental data. The calibrated DMN either allows to enrich real experimental data by virtual data and then to identify model parameters of anisotropic models or to carry out component simulations directly [3]. This work outlines the application of DMNs for highly non-linear deformation problems in the context of short glass fiber-reinforced polymers to industrially relevant problems.

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DATA-DRIVEN MULTISCALE FINITE ELEMENT SIMULATION AND ITS APPLICATIONS IN LITHIUM IONS BATTERIES

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ABSTRACT

As lithium-ion battery technology advances, a thorough comprehensive understanding of its performance and safety becomes increasingly imperative. This study focuses on a data-driven multiscale finite element simulation approach aimed at modeling and analyzing the intricate behavior of lithium-ion battery systems. To shed light on the multiscale interactions within the battery more comprehensively, we leverage experimental data to construct a data-driven constitutive model for electrode materials with considering the inhomogeneous effects of micro composite structures, capturing electrochemical-mechanical coupled behaviors. By integrating these models into a multiscale finite element framework, we can simulate and analyze the behavior of the battery across different scales, ranging from the particle to the macroscopic cell level. This holistic simulation approach facilitates a deeper understanding of the multiscale and multiphysical processes occurring within the battery. This study provides profound insights for the further optimization and enhancement of lithium-ion battery technology, holding significant implications for the future of renewable energy storage.

AN AUGMENTED LAGRANGIAN TRUST-REGION METHOD TO ACCELERATE CONSTRAINED SHAPE OPTIMIZATION PROBLEMS USING MODEL HYPERREDUCTION

Tianshu Wen[*1] and Matthew Zahr*[1]

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ABSTRACT

We present an augmented Lagrangian trust-region method to efficiently solve side-constrained optimization problems governed by large-scale nonlinear systems of equations. A globally convergent, hyperreduced trust-region framework is embedded in the nested optimization to ensure the global convergence of the overall framework towards the critical point. The trust-region framework constructs a hyperreduction model via empirical quadrature procedure (EQP) on the fly, which completely avoids an offline training phase. Two numerical experiments are performed on the shape optimization problem to verify and demonstrate the efficiency of the proposed work.

Phase-field modeling: Analytics, benchmarks, and discussions
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PARAMETRIZATION OF PHASE-FIELD MODELS FROM ATOMISTIC SIMULATIONS AND MECHANO-THERMAL CHARACTERIZATION

Frank Wendler[*1], Dilshod Durdiev[1], Michael Zaiser[1], Takahiro Tsuzuki[2], Hikaru Azuma[2], Shuji Ogata[2], Ryo Kobayashi[2] and Masayuki Uranagase[2]*

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[2]Nagoya Institute of Technology

ABSTRACT

Phase-field models are applied since more than three decades to a vast spectrum of microstructure related problems in materials science and engineering. The length scale spans the range of microscopic order parameters that decribe deformation and defects like twinning and dislocations on an atomic scale, over mesoscopic models for interface motion in grain growth or solid state transformation up to the scale of a polycrystalline sample, where coarse grained phase fields can be used.
In the talk we highlight the importance of a consistent parametrization for physically valid predictions for two problems on separate length scales:

For ferroelectric barium titanate (BTO), microscopic phase-field models based on the Landau-Ginzburg-Devonshire theory offer a bottom-up approach, where a comprehensive energy landscape can be generated from molecular dynamics simulations (MD). This proves particularly valuable for quantitatively incorporating defects into the continuum approach. Essential material parameters, including elastic and piezoelectric properties, kinetic coefficients, and domain wall characteristics, are extracted from MD data to refine the anisotropic gradient energy.
The polarization switching process in BTO involves localized nucleation and subsequent domain growth under the influence of an applied electric field. MD data establishes the significant role of thermal activation in domain nucleation, resulting in a notable scatter in observed parameter like the coercive fields. Utilizing this data, we develop a statistical method to calculate the activation parameters governing polarization switching at coercive fields, providing crucial insights into domain wall energy. This information is then used to parameterize the phase-field model.

On the device scale (~ mm) we present a model for martensitic transformation in shape memory alloys that is computationally tractable by coarse graining of the underlying crystallographic phases into volume fractions and tensorial eigenstrain. The model is based on continuum theory for mechanics and thermal transport implemented within a finite element framework, and a transition state theory approach for thermally activated kinetics. The mechanical part of the Gibbs free energy is formulated as a continuous multi-well potential that is calibrated with data from mechanical characterization experiments, digital image correlation and calorimetric characterization.

For both models parametric optimization techniques are applied to find a best fit for the overall thermo-mechaníc (-electric) behavior. We sketch how interfacial energies and fluctuations of the transformation barriers can serve as a link between the scales.

Advances in computational biomechanics and mechanobiology
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MULTISCALE FINITE ELEMENT MODEL OF CARDIAC GROWTH AND BAROREFLEX REGULATION

Hossein Sharifi[1], Mohammad Mehri[1], Kenneth Campbell[1], Lik Chuan Lee[2] and Jonathan Wenk[1]*

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ABSTRACT

The heart functions within a complex system that adapts its function to alterations in loading via several mechanisms. For example, the baroreflex is a short-term feedback loop that modulates the heart's function on a beat-to-beat basis to control arterial pressure. On the other hand, cardiac growth is a long-term adaptive response that occurs over weeks or months in response to changes in left ventricular loading. In this study, we investigate the impact of a baroreflex feedback loop on left ventricular growth in simulations of valve disease. To achieve this, we integrated the effects of a short-term baroreflex feedback loop and a long-term growth algorithm into a beating multiscale finite element model of the left ventricle. The baroreflex loop modulates the system from the molecular-level function of myofilaments up to system-level parameters, such as heart rate, to control arterial pressure [1]. Meanwhile, the growth algorithm responds to the altered stress level of the myocardium to drive long-term changes in the geometry of the left ventricle. Specifically, eccentric growth (chamber dilation) is driven by time-averaged passive stress in the myofibers, while concentric growth (wall thickening) is driven by time-averaged total stress along the myofiber direction over the cardiac cycle. Our integrated model replicates clinical measures of left ventricular growth in two types of valvular diseases - aortic stenosis and mitral regurgitation - at two different levels of severity for each case. Furthermore, our results showed that incorporating the effects of baroreflex control in simulations of left ventricular growth not only led to more realistic hemodynamics, but also impacted the magnitude of growth. Specifically, our results highlighted the role of regulating venous compliance (vasoconstriction) by the baroreflex immediately after the onset of valvular diseases, which has a significant role on the extent of LV growth in the long term.

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Modeling and learning of structured dynamical systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADAPTIVE CHOICE OF NEAR-OPTIMAL INTERPOLATION POINTS FOR STRUCTURE-PRESERVING MODEL REDUCTION

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[2]*Max Planck Institute for Dynamics of Complex Technical Systems*

ABSTRACT

For the efficient generation of accurate reduced-order surrogate models, interpolation-based techniques are well-established, effective approaches. Typical challenges for such methods are the automatic choice of good or even optimal interpolation points as well as a suitable size for the reduced-order model. An approach that tackles the first problem for linear, unstructured systems is the Iterative Rational Krylov Algorithm (IRKA), which computes optimal interpolation points by iterative updates solving small, linear eigenvalue problems resulting from the projection of the original system quantities. Considering the case of systems with internal (differential) structures, one could think of a similar iterative approach. However, the eigenvalue problems resulting from the projection of the corresponding transfer functions are nonlinear such that the number of potential new interpolation points exceeds the order of the reduced model. In our work, we propose StrAIKA (Structure-preserving Adaptive Iterative Krylov Algorithm), an IRKA-inspired iterative interpolation method for structured systems to compute near-optimal interpolation points as well as a suitable size for the reduced-order model. Thereby, the iterative updates of the expansion points are chosen to yield accurate approximations in specified frequency ranges of interest.

Advances in numerical methods for solution of PDEs
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SUMMATION-BY-PARTS FINITE-DIFFERENCE OPERATORS FOR SINGULAR COORDINATE SYSTEMS

Jonatan Werpers[*1]

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ABSTRACT

We present a general scheme for using existing summation-by-parts (SBP) finite-difference (FD) \cite{svard2014review} operators with singular coordinate transformations. The scheme preserves the accuracy and SBP properties of the original operators and permits simple implementation into existing codes.

The scheme allows taking advantage of the many previously constructed SBP-FD operators and developments when solving problems involving coordinate singularities. This greatly simplifies the design of the numerical method by avoiding re-constructing operators for the given coordinate system.

The operators are modified by viewing them in a weak form and eliminating the degrees of freedom associated with the coordinate singularities. By then returning to a strong form formulation an operator for the reduced grid is achieved which can be handled as any other SBP-FD operator.

Using the scheme we derive a stable and high-order accurate finite-difference method for underwater acoustic wave propagation in an axisymmetric domain. The method handles range and depth-dependent material properties, including discontinuous jumps. The accuracy and stability properties of the method are proven and corroborated using numerical experiments.

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@article{svard2014review,
  title={Review of summation-by-parts schemes for initial--boundary-value problems},
  author={Sv{\"a}rd, Magnus and Nordstr{\"o}m, Jan},
  journal={Journal of Computational Physics},
  volume={268},
  pages={17--38},
  year={2014},
  publisher={Elsevier}
}
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Advances in computational biomechanics and mechanobiology
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IPSC-DERIVED ENDOTHELIAL MULTI-CELL NETWORKS SYNERGISTICALLY MODIFY THEIR BASAL CONTRACTILITY MACHINERY AND EXTRACELLULAR MATRIX IN 3D

Toni West[1], Jiwan Han[1], Gabriel Peery[1], Robin Tuscher[1], Janet Zoldan[1] and Michael Sacks[1]*

[1]*The University of Texas at Austin*

ABSTRACT

INTRODUCTION: We have seen within 3D matrices that newly differentiated endothelial cells (ECs) from induced pluripotent stem cells (iPSCs) migrate towards each other and form networks of connected cells which configure into hollow tubes that resemble capillary networks, (Crosby et. al. 2019 Tiss Eng Part A). Understanding how the mechanical attributes of these cell networks change and affect their microenvironment is key to developing efficacious stem cell therapies for microvascular diseases. In our current work, we hypothesize that measurements from 3D traction force microscopy (3D-TFM) experiments can be implemented to develop inverse models to determine how networks of endothelial cells differentially affect their 3D microenvironment (through degradation and collagen deposition) and how their cytoskeletal structure organization is distinct compared to individual cells.

METHODS: We have previously developed a Gaussian process model to determine how basal cell contractility affects displacement of the surrounding 3D matrix through traction force microscopy (3D-TFM) and have developed an inverse computational model to depict localized cell-induced modification of the matrix modulus and an inverse computational continuum model of the internal stress fiber structure of single cells, (Sacks et. al. 2020 Biophys J; Khang et. al. 2023 J Biomech Eng). Our models therefore account for localized differences in modulus that previous 3D-TFM models assumed were homogenous. Since cells degrade extracellular matrices to grow and move in them while also depositing stiff matrix substances such as collagen, factoring the variation in matrix modulus into our calculations allows us to determine the cell-generated traction forces with much less error. Here we have further developed our models to determine the mechanical properties of nuclei, cells, and the microenvironment of 3D multi-cell networks from experimentally measured displacements that occur because of basal contractility.

RESULTS: From our computational models, we found that multi-EC networks, when compared to individual ECs, have roughly four times the strain energy per cell volume, an increase in extracellular matrix modification per cell volume, and differing stress fiber orientation that affects basal nuclear shape. These results suggest that networks of iPSC-EC cells synergistically work together mechanically to form capillary beds. The increase in strain energy per unit volume indicates that the cells are more energy dense as clusters. Further research into the mechanical properties of iPSC-derived ECs will enable understanding of how these cells are able to maintain structural integrity as they highly modify their environment, paving the way for development of stem cell therapies for microvascular diseases.

HYGROMECHANICAL MODELING OF FIBER REINFORCED POLYAMIDE ON MICRO- AND MACROSCALE

Paul Wetzel[*1], Benjamin Schneider[1], Jan-Martin Kaiser[1], Anna Katharina Sambale[2] and Markus Stommel[23]*

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[2]Leibniz-Institut für Polymerforschung Dresden e.V.
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ABSTRACT

In this study, the anisotropic hygromechanical behavior of short fiber reinforced polyamide 66 is modeled using numerical homogenization. For this, a solver based on the Fast Fourier Transform (FFT) is deployed on the microscale while finite elements are used on the macroscale.

On the microscale, the deformation behavior, including thermal and hygroscopic expansion, as well as the moisture diffusion process in the polymer matrix are studied. Based on micro-computed tomography (µCT) scans, representative volume elements (RVEs) of the 3D microstructure consisting of short glass fibers and a polyamide 66 matrix are generated. Next, an FFT-based solver operating directly on 3D voxel images is deployed [1]. Uniaxial tensile tests, thermomechanical analysis (TMA) as well as moisture sorption and swelling experiments are performed and used to calibrate the constitutive model of the polymer matrix [2]. After calibration, the present RVE simulations are capable of reproducing the key experimental findings.

On the macroscale, an anisotropic constitutive model is applied in finite element simulations. The model parameters are identified in advance using further RVE simulations that enrich the experimental test results with virtual test data for further loading directions and microstructure variations. The mechanical model features anisotropic elastoplasticity as well as thermal and hygroscopic expansion coefficients given as a function of the local moisture content, temperature and the state of fiber orientation. To solve the hygromechanical field problem, sequential coupling is used, i.e., first, the moisture diffusion problem is solved independently of the state of mechanical loading, and next, the resultant moisture concentration field is prescribed in the mechanical simulation. The capabilities of the macroscale model are shown in simulations of a demonstrator part which are verified against additional experiments.

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UNCERTAINTY PROPAGATION FOR MULTI-PHYSICS SIMULATION IN GAS TURBINE DESIGN

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ABSTRACT

The use of modeling and simulation in gas turbine design has increased substantially over the last few decades. However, computing key quantities of interest in gas turbine systems typically remains beyond the abilities of a single governing multi-physics simulation. Thus, 'analysis chains' must be linked together by separate specialty teams to obtain these outputs. This makes uncertainty propagation difficult, both technically and organizationally, often requiring judicious simplifications by technical experts to keep the computations to a tractable level. This talk considers steps towards epistemic uncertainty propagation in this setting, a model-centric treatment of uncertainty sources, and highlights the differences in separating sources of uncertainty through single and double-loop sampling.

Applications of shape optimization in complex engineering problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SHAPE OPTIMIZATION OF HYDRODYNAMIC EXPERIMENTS

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ABSTRACT

We are interested in shape optimization of hydrodynamic experiments, where the term “hydrodynamics” refers to the motion of solids and/or fluids under extreme conditions. Typically, the materials are solid at time t=0, but due to extreme pressure, temperature, and deformation the solid materials become fluid at later time. Examples of hydrodynamic experiments include high velocity impact, laser induced deformation, or explosively driven problems. A common theme in many hydrodynamic experiments is the existence of instabilities such as Rayleigh-Taylor (acceleration driven) or Richtmeyer-Meshkov (shock driven). The overall goal of our research is to answer the question: is it possible to optimize the shape of a material interface to either enhance or suppress a Richtmyer-Meshkov instability? In this work the material interface is parametrized by a few (< 10) parameters. The physics simulations are performed using a high-performance Arbitrary Lagrangian Eulerian (ALE) finite element code BLAST [1]. Since our ALE physics code cannot provide exact design derivatives, several alternatives were investigated: surrogate-based design optimization using neural network surrogate models, trust region Bayesian optimization, and gradient-based optimization using finite difference gradients. These algorithms were applied to the design of high-velocity impactor experiments [2] and explosively-driven shaped charges [3]. The advantages and disadvantages of these algorithms will be discussed in detail. Finally, physical experiments were performed to validate the designs.

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Towards predictive digital twins: Innovative algorithms for physics-, data-assisted and hybrid modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

REDUCING UNCERTAINTY IN DIGITAL TWIN MODELS: USING DATA CONSISTENT INVERSION TO BUILD POPULATION-INFORMED PRIORS FOR BAYESIAN INFERENCE

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ABSTRACT

Bayesian inference is essential to building predictive digital twins of physical assets as it incorporates information from observational data to reduce uncertainties. However, it is challenging to reduce digital twin uncertainty when relying solely on data from an individual asset. Consequently, this work presents an approach for utilizing data from a population of related assets to construct informative Bayesian priors that reduce uncertainty in individual digital twin asset. Specifically, we use data consistent inversion to construct population-informed priors using data on the population of related assets. We demonstrate this approach for a material mechanics model representing additively manufactured structures. Our numerical examples show that utilizing population-informed priors significantly increases the Kullback–Leibler divergence, i.e. the information gain, from the posterior to the prior in comparison to standard prior specification. These results are complemented with theory for linear-Gaussian inference that establishes the conditions under which using our approach is guaranteed to improve posterior estimates of uncertainty.

SPACE-TIME GALERKIN FINITE ELEMENT DISCRETIZATION AND ERROR CONTROL FOR COUPLED PROBLEMS

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ABSTRACT

In this talk, we discuss space-time discretizations with Galerkin finite elements for coupled problems. Therein, the temporal direction is discretized with discontinuous finite elements, while continuous finite elements are adopted for the spatial part. For us, space-time modeling is used to design goal-oriented error control with adjoint sensitivity weights, the same, as used for numerical optimization. Therein, a partition-of-unity is employed for error localization. For both, space-time discretizations and error control, we present recent advances in the treatment of nonstationary, coupled PDE systems.

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Biomechanics of hard tissues: From experiments and simulations to clinical applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EVOLUTION OF BIOMECHANICAL SIMULATIONS: VIRTUAL RECONSTRUCTION OF GENERATED FRACTURES

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ABSTRACT

Within the area of orthopedics and trauma surgery, precise classification and understanding of fractures play a crucial role in the development of effective treatment plans and favorable patient outcomes. The AO classification system has been categorized fractures based on anatomical location, severity, and specific fracture patterns [1]. Leveraging the AO classification method, we create virtual fractures, broadening the scope of biomechanical simulations and enhancing our insights into treatment options and healing processes. Crucial to the outcome of a biomechanical simulation is the bone model itself. Clinical image data is scarce or of poor quality, significantly are impacting the results of the simulations. To circumvent this issue, Geomagic FreeformTM software is used. Furthermore, one could extend the virtual reconstruction and use a statistical shape model as a base and implement the fracture pattern. Our approach aims to foster a comprehensive understanding of fracture patterns, their biomechanical implications, and the potential of virtual reconstruction to enhance diagnostic and therapeutic strategies. The workflow comprises the following steps: (1) Utilizing freeform software and its specialized modeling tools to generate various fracture types in pre-existing bone model from clinical image or generate the fracture in a statistical shape model. The bone is now divided into three bone segments: distal and proximal bone segments and the fracture itself. (2) Assigning material parameters to individual segments and passing the bone to a high-quality finite element mesh generator. (3) Biomechanical simulation involves defining subject-specific boundary conditions and applying the joint force to the according bone segment. The required joint force is derived from our monitoring database. Braun et al.[2] outlines the procedure for a distal tibial shaft fracture. Similarly, the calculation of arbitrary joint forces can be approached. By blending virtually generated fractures with subject-specific boundary conditions, we can create a diverse array of pertinent biomechanical simulations, thereby enriching our understanding of the fracture's biomechanics. The use of freeform software for biomechanical simulations open new dimensions for research, promising a deeper understanding of fracture geometries and their clinical implications.

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Data-driven approaches for solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-ADAPTIVE MODELING OF HYPERELASTIC CONSTITUTIVE LAWS: APPLICATION TO EXTREMELY SOFT MATERIALS

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ABSTRACT

The traditional approach to modeling the non-linear constitutive behavior of soft materials at finite strains relies on hyperelasticity, a paradigm that inherently involves uncertainties in phenomenological constitutive modeling. This method often results in information loss since experimental data is not directly integrated into calculations, and the engineer's selection of a suitable strain energy function heavily depends on experience.

In contrast, data-driven approaches present a promising alternative. We recently introduced an innovative data-adaptive approach for modeling hyperelastic materials at finite strains [1] allowing for more efficient inclusion of experimental data. The proposed modeling procedure ensures adherence to crucial constraints such as thermodynamic consistency, material objectivity, frame indifference, and material symmetry a priori.

The fundamental concept involves formulating an approximation of the strain energy function using a sum of basis functions multiplied by parameters. The basis functions are expanded over the space of invariants, and support points, where the parameters are defined, are distributed in the invariant space. These parameters are determined through a nonlinear optimization problem, minimizing the 2-norm of the residual vector, representing the difference between measured and computed displacements and reaction forces. Importantly, our approach does not depend on measured stresses, setting it apart from many existing data-driven and model-free methods.

In our initial investigation, we demonstrated the efficiency and flexibility of our method based on numerical experiments and linear finite-element-like basis functions. The focus of this contribution is on the applicability to real experimental data obtained from Digital-Image-Correlation and basis functions with higher continuity. Specifically, we concentrate on a substantial experimental database encompassing various soft materials, particularly ELASTOSIL, VHB, and DOWSIL, with the aim of identifying a set of strain energy functions characterizing these materials in a fully automated and reliable manner.

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Fluid dynamics and SciML: Navigating challenges and seizing opportunities
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

UTILIZING SUPERVISED MACHINE LEARNING TO ENABLE DYNAMIC ADAPTIVE SUBGRID MODELING FOR MULTISCALE HYBRIDIZED FORMULATIONS

Tim Wildey[*1]*

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ABSTRACT

Multiphysics systems are often strongly coupled, highly nonlinear and characterized by multiple physical phenomena that span a large range of length- and time-scales. Performing direct numerical simulation of such systems that resolves all the relevant length and timescales is often prohibitive, even on the modern leadership-class computing platforms. Nevertheless, these fine-scale variations often impact the behavior of the system on a much larger scale in non-negligible ways. Thus, one often seeks to model or approximate the subgrid scale phenomena to accurately and efficiently capturing their impact on the coarse scale solution. Multiscale formulations based on non-overlapping domain decomposition methods can be viewed as variational multiscale methods and have the additional benefit of allowing different physical models and numerical discretizations in different regions. However, determining the optimal subgrid model within a coarse scale region that effectively balances accuracy and computational expense can be challenging for transient nonlinear multiphysics applications.

In this presentation, we describe our theoretical and computational frameworks that are based on a generalization of hybridized discretizations and are designed to exploit heterogeneous computational architectures to enable concurrent multiscale modelling on a range of transient nonlinear multiphysics applications. We will also describe our utilization of dynamic adaptive subgrid modelling and how we are utilizing supervised machine learning strategies to determine the appropriate subgrid model for an element in the coarse scale partition. We will provide demonstrations on applications motivated by subsurface flow and mechanics in porous media and additive manufacturing.

Certification of simulations and model adaptation in computational science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HP-ADAPTIVE SPARSE GRID COLLOCATION METHODS FOR UNCERTAINTY QUANTIFICATION IN GAS NETWORKS

Hendrik Wilka[*1] and Jens Lang*[1]

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ABSTRACT

In this talk, we present a newly developed hp-adaptive method for uncertainty quantification which arises in the simulation of gas transport problems on networks. In short-term optimal control problems, the isothermal Euler equations are used in combination with uncertain boundary data caused by varying demands of consumers. Here especially the pressure is of interest since it should stay in given bounds with a high probability [1]. In recent works, global sparse grid methods have been applied to overcome the curse of dimensionality when approximating functions in high-dimensional probability spaces [2]. As investigated in [3], kinks can arise in important quantities of interest, e.g. for the maximum pressure over a time interval. This leads to well known difficulties when global polynomials of higher order are used. To also approximate non-smooth functions, we have developed a novel sparse grid collocation approach that uses local polynomials with a restricted support as basis functions. This allows us to place additional collocation points in regions where the error is over a predefined threshold. In contrast to previous works, our method is hp-adaptive: In smooth regions, the polynomial degree of the basis functions is increased (p-refinement), while low-degree polynomials are used near kinks (h-refinement). We present two refinement strategies. The first one is a greedy approach which chooses those basis functions having the smallest interpolation errors at new collocation points. A second strategy uses a kink detection algorithm to limit the polynomial degree in non-smooth regions. We discuss academic problems from the Genz test function package as well as examples for gas networks where kinks in pressure functionals are present. We compare our method with other approaches.

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Computational particle-based solvers for multiphysics & multiscale simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VERIFYING DISCRETE ELEMENT MODELS THROUGH MICROMECHANICAL ANALYSIS OF FORCE AND TRACTION CHAINS

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ABSTRACT

Discrete Element Modeling (DEM) has emerged as a tool for understanding and predicting granular materials' behaviour and micromechanical state in various engineering and scientific contexts. This study extends an innovative approach to calibrating DEM simulations by utilising micromechanical concepts [1], specifically focusing on verifying models from force and traction chains within granular assemblies. The verification process involves a detailed statistical analysis of force chains, providing a robust framework for assessing deterministic and non-deterministic DEM codes.

At the core of this approach is the examination of force chains, which are networks of interconnected particles transmitting forces through contact points in granular materials. These chains form the fundamental structural backbone of granular assemblies, dictating their mechanical response under different loading conditions. By analysing the properties and distribution of these chains, we can gain insightful information about the micromechanical state of the material. This method quantifies key characteristics such as chain length, orientation, intensity, and spatial distribution. Traction chains offer insights into the surface interactions between particles. They are critical in understanding the frictional and adhesive forces at play, which are essential in the realistic modelling of granular materials. The analysis of traction chains complements that of force chains by providing a more comprehensive understanding of the micromechanical interactions within the material.

Statistical tools are included to analyse micromechanical elements within DEM simulations. This statistical approach accommodates deterministic and non-deterministic codes, allowing for evaluating models with inherent randomness due to random execution with limited numeric precision. The statistical analysis involves comparing theoretical and numerically verified and validated models against theoretical and validated ones, thereby assessing the accuracy and reliability of the DEM simulations. This verification process serves as an ‘acceptance testing' strategy for DEM codes, ensuring that the fundamental micromechanical behaviours are accurately captured before applying the model to more complex scenarios. Such rigorous testing is crucial for enhancing confidence in DEM simulations, which are increasingly used to predict material behaviour in applications ranging from pharmaceuticals to civil engineering.

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Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FROM TICOM TO THE ODEN INSTITUTE: THE VISIONARY LEADERSHIP OF J. TINSLEY ODEN

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ABSTRACT

In 1973, J. Tinsley Oden joined the faculty of The University of Texas at Austin. Over a series of conversations with colleagues, he saw the opportunity to use computing to solve engineering problems and he saw the need to pull people together. He said: “One day it hit me, this is where the world is going - concepts in computers and solving problems in physics, mathematics, and mechanics. I saw the need to pull them all together into a unified approach.” That led him to establish the Texas Institute for Computational Mechanics (TICOM) in 1973. Under Oden's leadership, TICOM played a critical role in the founding and advancement of the field of computational mechanics. Fifty years later, TICOM has grown to become the Oden Institute for Computational Engineering and Sciences. From TICOM to the Oden Institute, this talk will give a brief history of J. Tinsley Oden's 50-year visionary journey of leadership, mentorship, and service at UT Austin.

Emerging frontiers and methods in digital manufacturing: Modeling, simulation, and beyond
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOWARDS A MULTISCALE COMPUTATIONAL FRAMEWORK FOR SIMULATING FLOW-MEDIATED CRYSTALLIZATION BASED ON PHASE-FIELD CRYSTAL FORMALISMS

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ABSTRACT

Liquid-solid phase transitions into crystalline solids are ubiquitous in industries ranging from additive manufacturing to pharmaceutics to surface coating processes. One system, in particular, CsPbI_3 perovskites, exhibits disparate solar harvesting properties under different crystal structures. Crystal microstructural control and defect prevention during processing is a huge challenge with further complexities arising from coating flows of solar cells for mass production.

With limited experimental techniques to observe flow-mediated crystallization in situ, it is paramount to gain insight from first-principle aware simulations for understanding and controlling crystallization kinetics and phase stability mediated by flows. In this work, we demonstrate the development of a multiscale and multiphysics computational framework for simulating flow-mediated crystallization based on phase-field crystal (PFC) formalisms. Compared to traditional molecular dynamics, which are limited to small spatiotemporal scales, and phase-field methods (e.g., Allen-Cahn), which neglect crystal-level information, we aim to develop a multiscale computational framework that connects crystal-level information to macroscale phase behavior in the presence of flow.

We validate our model by reproducing existing perovskite crystal structures under varying conditions from experiments and course-grained molecular dynamics. We then introduce how we incorporate the effect of flow on crystal structure. Strategies for controlling the crystal microstructure through computation-driven processing conditions will also be discussed in the spirit of digital manufacturing.

Computational modeling of extreme-loading events
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN ASSESSMENT OF THE APPLICABILITY OF MODERN RKPM METHODS TOWARDS SIMULATION OF CONCRETE UNDER EXTREME EVENTS

Dominic Wilmes[1], Michael Hillman[1] and Joseph Magallanes[1]*

[1]*Karagozian and Case, Inc.*

ABSTRACT

Due to its widespread usage in a variety of vital structural applications and infrastructure, the safety and performance of concrete under extreme events, such as impact or blast, is essential to understand and be able to calculate in a predictively. Towards this end, a number of constitutive models have been developed which seek to capture the wide range of behaviors present in concrete such as those related to hardening, softening, rate effects, fracture, etc. However, these material models only comprise a portion a of a given physics-based numerical analysis as they generally represent a discrete material point in a larger numerical framework. As a consequence, capturing large scale discontinuous phenomenology of concrete response such as fracture, fragmentation, scabbing, and spall are often dependent on the numerical framework the material model is embedded in.

In this work, the advantage of utilizing meshfree methods to provide this robust numerical framework for treating concrete under extreme events will be demonstrated using problems which demonstrate a wide range of concrete phenomenology. A series of concrete benchmark problems will be compiled which seek to show several types of phenomenology found within problems involving concrete materials. A modern RKPM [1] numerical code, KC-FEMFRE, will be applied to each of these benchmarks and the results and efficiency from running these benchmarks will be documented compared against previous results taken from open literature, widely-used commercial solid mechanics codes, and experimental results, when applicable. To ensure fair comparison between existing solvers, the K&C Concrete model [2] will be leveraged as a VUMAT in all simulation codes utilized in this study. This will alleviate any differences that might be constitutive model implementation specific and demonstrate applicability of meshfree for this problem domain against comparable options.

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ACCUMULATED EPISTEMIC UNCERTAINTIES AND THE CHALLENGE TO QUANTIFY THEM IN MULTIPHYSICS PREDICTIONS

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ABSTRACT

Epistemic uncertainties are inherent to computational physics and can be introduced at every level of the computational model development process. Sources include systematic errors in experimental measurements, model-form errors, errors due to algorithmic and numerical choices, and interpretation of the active mechanisms in a multiphysics process. Epistemic uncertainties can arise from a lack of understanding of the physics – both mathematically or phenomenologically - or out of the necessity to reduce computational expense.

Epistemic error sources can be particularly challenging to diagnose with common statistical methods because of their non-probablistic nature. This is particularly true for predictive multiphysics simulations for which many epistemic errors accumulate in integral multiphysics simulations and quantities of interest. This conglomeration of correlated, uncorrelated, and/or, possibly, mutually exclusive epistemic uncertainties is observed across computational physics disciplines and necessitates collaborative consideration of approaches across disciplines.

In this talk, I will discuss specific epistemic uncertainties observed at Los Alamos National Laboratory, specifically focusing on the concept of accumulated epistemic uncertainties. These examples will be used to 1) motivate the discussion of epistemic uncertainty management and 2) encourage the need for collaboration across computational disciplines toward engineering and statistics methods for quantifying epistemic uncertainties.

Lattice Boltzmann modelling and study of complex flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A PYTORCH BASED FULLY DIFFERENTIABLE LATTICE-BOLTZMANN SOLVER FOR HYBRID MACHINE LEARNING SIMULATION WORKFLOWS

Josef Winter[*1], David Wawrzyniak[1], Steffen Schmidt[1], Thomas Indinger[1], Christian Janssen[2], Uwe Schramm[2] and Nikolaus Adams[1]*

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ABSTRACT

Researchers are successfully exploring the concept of differentiable simulators that solve the governing equations of fluid mechanics [1]. Differentiable simulators are gaining prominence due to their applicability across various scientific fields, ranging from the design of data-driven numerical models to reinforcement learning and novel concepts hybridizing simulation and machine learning (ML) workflows. They exploit that numerical methods frequently involve computing the output of discretized operators, which can be divided into sequentially linked elementary units akin to the sequential design of numerous ML architectures. The key features of differentiable simulators include their ability for gradient calculation via automatic differentiation, the integration of ML within simulation workflows, and enhanced computational efficiency when executed in ML frameworks equipped with powerful acceleration features.
We present a PyTorch-based implementation of the Lattice-Boltzmann method (LBM). The LBM is a highly flexible and reliable solution for challenging computational fluid dynamics simulations, renowned for its exceptional parallel efficiency. Our implementation leverages modern software design principles to compose the LBM algorithm from sequentially connected modules. This design ensures seamless compatibility with programming paradigms of PyTorch and allows efficient usage of GPU accelerators. The application programming interface of the solver relies on principles commonly used by ML libraries to fully streamline hybrid workflows.
Based on this modular code design, we provide algorithmic building blocks for various velocity sets, collision models, and boundary conditions that can be interchanged flexibly without losing performance. Additionally, we provide modules for simulating complex multi-phase flow phenomena.
We illustrate the smooth interplay of numerical simulator and ML building blocks by constructing surrogates for complex flow problems using state-of-the-art ML models such as Fourier Neural operators. These models are particularly attractive for their discretization invariance and capability to facilitate zero-shot super-resolution. Also, we present a hybrid approach that merges learned operators capturing the dynamics of the simulation with the numerical simulation. Our approach advances parts of the overall simulation using the learned operators instead of the numerical schemes. Thereby, we drastically reduce the computational cost of the simulation.
The results demonstrate the immense potential of integrated ML simulation workflows, especially in enhancing the efficiency of numerical simulations using the Lattice-Boltzmann method. The careful design of our software framework eases the rapid development and deployment of such novel methodologies.

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Computational methods in environmental fluid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMPLEMENTATION OF SUBGRID APPROACHES ACCOUNTING FOR UNRESOLVED TOPOGRAPHY IN AN ARBITRARILY-STRUCTURED C-GRID SHALLOW WATER FLOW MODEL

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ABSTRACT

In coastal inundation simulations based on numerical solution of shallow water equations, faithfully representing topography and bathymetry at high enough grid resolution is known to be a crucial factor in obtaining accurate results. However, in practice, a compromise in the grid resolution is often needed to made to a certain level because of a constraint in computing time. As a result, a predictive capability of the model may suffer especially in inundation and recession zones of flow in previously-dry and wet areas. In this work, we present an implementation of subgrid techniques accounting for unresolved topography in a single layer mode of the Model Prediction Across Scales-Ocean (MPAS-O), a finite-volume based method on staggered arbitrarily-structured C-grids. Numerical experiments using a set of test cases with wetting and drying, ranging from an idealized test problem with an analytical solution to a realistic test case of storm surge, demonstrate that the subgrid method can substantially improve the predictive capability of the MPAS-O coarse-grid simulations with only a minor increase in the computing time.

Architected materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GENERALIZED DATA-DRIVEN MATERIAL MODEL OF 3D-PRINTED BIAXIAL WEAVES USING TRANSFER LEARNING

Marc Wirth[*1] and Kristina Shea*[1]

[1]*ETH Zurich*

ABSTRACT

3D-printed weaves are versatile structures due to their unique combination of pliability, strength and tunability by design. The 3D-printing process enables tuning the weaves mechanical properties by modifying aspects of the weave design, such as the interlacing structure, the yarn geometry and the yarn material. This allows for the tuning of both the overall mechanical properties of the fabric and the local mechanical properties within the structure. For computational design of 3D-printed textiles with locally tuned mechanical properties, a rapid simulation utilizing a design-sensitive material model is key. Previous work has shown a model-free simulation approach of 3D-printed biaxial weaves approximated as planar truss structures utilizing a neural network as a surrogate model. The neural network is trained on the constitutive manifold of a discrete set of input samples varying in their weave design. Despite the versatility in depicting the mechanical behavior of weaves with different designs, the surrogate is limited in the generalization capabilities by the samples provided in the input set. This is a limitation to overcome, since 3D-printed architected structures are prone to change in their structural behavior due to variations in the manufacturing process, such as the manufacturing device and material batch used, and changes in the sample design. Here, we show the capability of the neural network based surrogate model to generalize for unseen samples by transfer learning. We enhance the constitutive manifold by samples varying from the initial input set in their design and printer type used for production and re-train the neural network on the new manifold. We evaluate the performance of the network when used for the simulation of samples having gradually varying designs and samples with designs not included in the manifold. We evaluate the performance when both interpolating and extrapolating in the design space of the samples constituting the constitutive manifold. We show the capability of a neural network utilized as a surrogate in model-free FE simulations to be beneficial in generalizing to new cases, which is especially useful when introducing new design variables and new 3D-printing methods, which would usually require extensive material characterization. With these results, we show the usage of a generalized material model for a large range of 3D-printed biaxial weaves, which enables the computational design of architected textiles.

GENERALISED FINITE VOLUME METHODS - TAYLORED TEST SPACES FOR INTERFACE PROBLEMS

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ABSTRACT

We present a fully-implicit and stable finite element and finite volume scheme for the simulation of freely moving particles in a fluid. The developed method is based on the Petrov-Galerkin formulation of a vertex-centered finite volume method on unstructured grids. Identification with a corresponding finite element bilinear form finally enables the derivation of a finite element method for particulate flow. Appropriate extension of the ansatz and test spaces lead to a formulation comparable to a fictitious domain formulation. In contrast to most fictitious domain methods no additional Lagrange multipliers or artificial external forces need to be introduced for the fluid-solid coupling. The interface forces are implicitly imposed through the original bilinear form for the fluid. The surface integrals of the finite volume scheme enable a natural incorporation of the interface forces. The extended scheme treats the particles as rigid fluid and the resulting system of equations does not possess saddle-point structure. As a result, only one single solve for the derived linear system for the fluid together with the particles is necessary and the proposed method does not require any fractional time stepping scheme to balance the interaction forces between fluid and particles. For the linear Stokes problem we will prove the stability of both schemes. Moreover, for the stationary case the conservation of mass and momentum is not violated by the extended scheme, i.e. conservativity is accomplished within the range of the underlying, unconstrained discretisation scheme. The scheme is applicable for problems in two and three dimensions.

Catastrophic failure mechanics and numerical modelling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL ANALYSIS OF CRASHWORTHINESS CONCEPTS FOR HYDROGEN-POWERED AIRCRAFT IN THE EARLY DESIGN PHASE

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ABSTRACT

Sustainable aviation has become a very active field of research. One promising approach are hydrogen-powered commercial aircraft. Many concepts for such aircraft have been published (e.g. [1]), but crashworthiness aspects are often neglected in the early concept phase.

Our research focuses on conventional configuration aircraft. As the volumetric energy density of hydrogen is only approximately one fourth of kerosene, the needed fuel volume is much higher. Most concepts therefore propose cryogenic liquid hydrogen (LH2) tanks inside the fuselage to provide the needed capacity. These large tanks close to the passenger cabin can pose a serious safety hazard in case of uncontrolled leakage or damage. A crashworthiness assessment is therefore viable to the whole concept, to meet the required high safety level of modern aircraft.

In the early design phase with its large parameter space, numerical simulations are an established possibility to investigate the behaviour during survivable crash scenarios. The challenges of performing such simulations with the available data are already discussed in literature (e.g. [2]). Current approaches mainly focus on the physical integrity of the passengers due to the accelerations during impact. Technically, they create high-fidelity finite element models from preliminary aircraft data, enriched by knowledge from existing aircraft constructions. Due to the high non-linearity and the large deformations during crash events, the models need to be granular enough to capture the major physics but also efficient enough to be applicable in an early design phase.

We want to present our progress in using such approaches to evaluate a crashworthiness concept build out of discrete crash absorbers to ensure the structural integrity of LH2-tanks during a crash scenario. One challenge is the different airframe architecture of fuselage sections with LH2-tanks. Due to the size, the cargo-deck and passenger-crossbeam are missing, rendering classical crashworthiness concepts used for passengers inapplicable. As the tanks are located close to the bottom, the fuselage kinematics must be influenced in a way that structural parts do not pierce the tanks.

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Computational models and methods for predicting cancer progression and treatment response
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SPATIO-TEMPORAL OPTIMIZATION OF THERAPUETIC CELL DELIVERY WITH DIGITAL TWINS

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ABSTRACT

Therapeutic cell therapies, such as CAR-T therapy, are a rapidly progressing methodology for treatment of tumors, and have shown broad success in "liquid" cancers. While theoretically effective for the treatment of solid tumors, many practical barriers exist, preventing widespread success of the method. This is especially the case for neurological tumors, where the blood brain barrier prevents uptake of therapeutic cells by the tumor. To overcome this challenge, some CAR-T trials have adopted the strategy of intratumoral delivery, placing cells directly in the treatment site using a surgical catheter. This strategy, while allowing for a higher dose of therapeutic cells in the target region, does not allow for subsequent placement of the catheter for repeat doses. As such, it is important that the catheter is placed optimally to ensure each dose of therapeutic cells provides as much benefit to the patient as possible. In this work, we present an image-informed model of therapeutic cell transport, capturing directed cell migration along fluid streamlines, and predator-prey-like dynamics. Spatial transport parameters are informed by the novel analysis method for dynamic contrast-enhanced MRI, known as LCFR. Cell growth dynamics are informed by a multi-species predator-prey-like model discovered by Brummer et al. (2023) using the SINDy methodology. Using this spatio-temporal multi-species model of therapeutic cell dynamics, we then optimize the delivery location and timing strategy for delivery of therapeutic cells for individuals, testing multiple temporal delivery strategies, and spatially optimizing catheter placement. This is done to encourage spread into invasive tumor margins, where non-enhancing tumor may be present, but undetectable by MRI. In preliminary study, we performed a forward simulation, sampling delivery locations at each 500 um in the x and y directions. We find that optimizing the delivery location within the 2D plane increases the total amount of tumor cells killed by a factor of 2.4 (maximum tumor cell kill/mean tumor cell kill), and simultaneously maximizes the total number of CAR-T cells present in the tumor between doses by a factor of 2.8 (maximum temporally-averaged CAR-T population/mean temporally-averaged CAR-T population). Using this strategy, we aim to give each individual patient an optimal surgical procedure, maximizing the potential efficacy of this treatment strategy.

Mesh-free particle methods for multi-physics problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DIFFERENTIABLE PROGRAMMING OF SMOOTHED PARTICLE HYDRODYNAMICS: COMPRESSIBILITY AND SHOCKS

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ABSTRACT

Many formulations of Smoothed Particle Hydrodynamics (SPH) have been developed for modeling compressible flows involving plasma, such as those seen in astrophysics and engineering applications. Often, these formulations are first tested and developed on simple flows, such as 1D and 2D shock problems in order to validate the modeling and numerical implementations. However, the parameters of these formulations are usually adjusted by trial and error. In this work, we explore the physics informed machine learning methods for finding these parameters. Thus, we develop a compressible SPH formulation consistent with differentiable programming in order to first learn the standard SPH parameters and then to find new parameterized terms such as smoothing kernels, artificial viscosity, and heat conduction, with the goal of improving the SPH framework with respect to accuracy and performance.

The approach is first validated and analyzed for the 1d Sod shock and 2D Taylor-Sedov blast wave problems, i.e. learn-able and parameterized compressible SPH formulations are fit to the analytical solutions using gradient based optimization. Next, we extend the SPH formulation to model the spatio-temporal evolution of plasma plumes generated from rapid thin-target heating by 20 MeV electron beams. The generation of plasma plumes during such heating processes can significantly impact various high-energy physics experiments, making accurate prediction of their behavior crucial for experimental design and analysis. The plasma plumes of interest evolve in vacuum, making the SPH framework a natural choice for modeling at the coarse grained scales of interest. Furthermore, the complex physics involved motivates the use of machine learning to fill in the gaps with exploring new parameterized terms within SPH. We employ experimental data to develop a hierarchy of SPH models, using pulsed bunches of approximately 10^{15} electrons to heat a range of thin targets to temperatures above 1 eV. The shadowgraph and interferometer measurements provide spatially resolved snapshots of the expanding plume's electron density and temperature distributions at discrete time points.

Recent advances in high-order methods for computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFICIENT HIGH-ORDER ENTROPY-STABLE DISCRETIZATIONS OF THE EULER AND NAVIER-STOKES EQUATIONS ON SIMPLICIAL ELEMENTS

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ABSTRACT

The summation-by-parts (SBP) framework enables construction of high-order entropy-stable discretizations of the Euler and Navier-Stokes equations. Although they have been shown to be more robust, these discretizations are substantially more expensive than the divergence form implementations of the equations, particularly on simplicial elements, which are favored for mesh generation around complex geometries. Their larger computational cost can be attributed to two-point inviscid flux computations, interpolation and change of variables, and computation of viscous flux Jacobian terms. The number of nodes in an element and their placement play an important role in the efficiency of entropy-stable discretizations, and any set of nodes amenable for construction of SBP operators must define a sufficiently accurate positive-weight quadrature rule. We seek operators that have as few nodes as possible for a given degree and with a subset of nodes placed at the element boundaries to facilitate efficient computation of numerical fluxes. In light of this, we present novel quadrature rules for construction of SBP diagonal-E operators offering, in many cases, fewer nodes than existing rules. We combine the Levenberg-Marquardt and particle swarm optimization algorithms to solve the quadrature accuracy conditions, addressing the challenges of finding good initial guesses and slow convergence rates. Positive weight and nodal symmetry constraints are enforced to find fully symmetric positive-weight quadrature rules. Furthermore, the range of suitable quadrature rules for SBP diagonal-E operators is significantly extended to encompass higher degrees. The cost of the inviscid fluxes is further reduced by constructing sparser SBP derivative operators, leveraging the presence of free variables due to the larger number of nodes than polynomial basis functions required to construct the operators. Finally, the inviscid flux discretization with the newly derived operators is combined with SBP-Ω type operators in a staggered grid formulation to reduce the cost of the viscous fluxes. We demonstrate the numerical properties of the proposed operators through test cases involving the Euler and Navier-Stokes equations.

ON A SPACE-TIME FORMULATION USING VIRTUAL ELEMENTS

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ABSTRACT

The virtual element method (VEM) for elasticity in solid mechanics was first considered in Beirao da Veiga et al. (2013). The possibility of VEM to construct of elements with arbitrary shape and arbitrary number of nodes has many ad-vantages in engineering. Thus, applications of the virtual element method were investigated in areas like finite strains, inelastic materials, contact and phase field approaches, see e.g. Wriggers et al. (2023). Another advantage is that virtual elements can be easily incorporated in classical finite element codes since they have the same number of unknowns.
So far, VEM has not been applied to space time formulations for structural el-ements like strings, trusses and beams. Here we develop a virtual element dis-cretization scheme that is suitable for dynamic applications. It is based on a space time formulation that is build upon the Hamilton principle and avoids the used of mass matrices. It will be shown that the developed elements outperfom finite elements in certain applications.

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Multi-scale, multi-rate damage and fracture: Models, experiments, and simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPLOSIVE FRAGMENTATION OF ADDITIVELY MANUFACTURED STAINLESS STEEL

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ABSTRACT

Properties of fragmentation from an explosively driven 316L stainless steel spherical shell section fabricated by a laser powder bed additive manufacturing process with minimal surface finishing are investigated. This shell is driven by an insensitive high explosive, resulting in high strain rate deformation (>8000/s) and failure of the stainless steel. Photonic Doppler velocimetry measures the expansion rate; dynamic radiography and high-speed imaging capture the fracture behavior of the stainless steel. The fracture response of the additively manufactured stainless steel shell is compared to published experimental results on additively manufactured 316L stainless steel and conventionally manufactured wrought 316L and 304 stainless steel shell fragmentation. Despite preferred crack orientation, suggesting the influence of surface grooves on fracture time, fragment size is identical to that measured in a similar experiment on wrought 304 stainless steel. Further analysis indicates that the 316L additively manufactured stainless steel shell exhibits comparable spall strength and fragmentation toughness to conventionally manufactured stainless steel yet lower failure strain due to surface stress concentrations.

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Computational methods in environmental fluid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LARGE-EDDY SIMULATION OF INTRUSIVE GRAVITY CURRENTS AT RIVER CONFLUENCES

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ABSTRACT

River confluences, a ubiquitous feature in catchment areas, play a crucial role in all fluvial networks. The complexity of flow characteristics at these junctions arises from the three-dimensional nature of the flow, attributed to tributary convergence and potential sediment transport, leading to variations in depositional areas and bed topography. Generally, gravity currents emerge as the primary driving mechanism, given their substantial interactions with the underlying bed material and ambient fluid. To grasp the intricacies of transport processes, it is essential to understand the evolution of flow morphologies and the dynamics of gravity current propagation. While numerous studies extensively explore the morphodynamics of individual channels, sinuous submarine channels, and river confluences, documented through field observations, laboratory experiments, and depth-averaged numerical models, relatively less attention has been devoted to investigating three-dimensional gravity currents intruding into the main channel under constant inflows. In this study, our aim is to gain insights into the flow dynamics of gravity currents at river confluences through large-eddy simulations. The primary controls influencing the magnitude of river morphology are identified as the ratio of driven velocity between the mainstream and the tributary and their junction angle. This study addresses several key discussions, including (1) flow morphologies, (2) flow structures, and (3) the relationship between baroclinic pressure gradients and shear layers.

Mechanobiology of cells, vesicles and biomembranes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING CELL ADHESION AND SPREADING MEDIATED BY LIGAND DIFFUSIVITY

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ABSTRACT

Cells live in a dynamic environment where their physical connections and communication with the extracellular matrix (ECM) are mediated by receptor-ligand binding. Therefore, a precise knowledge of receptor-ligand interactions is crucial for comprehending cellular behaviors. Interestingly, recent evidence has suggested that the mobility of ligand molecules at the cell-ECM interface significantly affects cell adhesion and spreading, although the underlying mechanism remains elusive. In this study, we employed a modeling approach to address this critical issue. Specifically, we adopted Langevin dynamics to simulate the random movement of ligands by assigning a stochastic force along with viscous drag. We then analyzed the evolution of cell adhesion and subsequent spreading by considering the force-regulated binding and breakage of molecular bonds connecting polymerizing actin bundles inside the cell to the ECM. Notably, our results predicted a biphasic relationship between cell adhesion and ligand diffusivity, with maximal cell spreading occurring at intermediate ligand mobility. Furthermore, we found that the peak position was influenced by ligand aggregation, which effectively reduced their diffusivity and the kinetics of bond association/dissociation. These predictions were in excellent agreement with our experimental observations, where ligand mobility was manipulated by tuning the interactions between the self-assembly polymer coating and the surface.

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Immersed-boundary variational methods: Theory, data structures, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AGGREGATED UNFITTED FINITE ELEMENT METHOD FOR FULLY COUPLED POROELASTICITY

Fanke Wu[*1], Wenquan Yuan[1], Chenguang Li[1], Yongwei Wang[2] and Zhijun Liu[1]*

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ABSTRACT

Complex boundaries and material interfaces are common in scientific and engineering problems. When solving such problems with the standard finite element method (FEM) where the elements conform to boundaries and interfaces, analysts have to pay great efforts and patience for the meshing to avoid low-quality elements in the vicinity of boundaries and interfaces. Therefore, meshing or preprocessing is normally time-consuming and arduous for practical problems. The unfitted FEMs provide another path for the solution of problems with complex geometric domains, where a simple mesh not necessarily aligning to the physical model is employed. However, the boundaries and interfaces can cut the mesh and produce tiny cut elements, which causes ill-conditioning of the stiffness and mass matrix. The recently developed aggregated unfitted resolved the cut-induced ill-conditioning by linking the unknowns of nodes outside the physical domains to the adjacent nodes within the physical domain. It did not introduce any additional stability terms and, therefore, maintained the consistency. Hence, it is more favorable than stabilized unfitted FEM when consistency is desired.

The majority of geotechnical problems often involve complicated external boundaries and material interfaces. Therefore, the aggregated unfitted FEM is an excellent tool for analyzing geomechanics and geotechnical problems. In this paper, we develop an aggregated unfitted FEM for hydro-mechanical coupling problem, which is one of the most important problems in geomechanics. In the development of this methodology, we link both the displacement and pore pressure of nodes located outside the physical domain to the nodes inside the physical domain via extrapolation. The ill-conditioning is avoided as the small cut supports of the nodes outside the domain are precluded. Several benchmark hydro-mechanical coupling problems are solved with the proposed aggregated unfitted FEM. The numerical experiments demonstrate the optimal spatial and temporal convergence regardless of how the meshes are cut. Furthermore, the condition numbers of the stiffness matrix are dependent of the smallest cut ratio.

Multi-scale and machine learning-based modeling methods for optimization and design of composites
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

OPTIMIZATION DESIGN METHOD FOR HIGH-ASPECT-RATIO COMPOSITE WING BASED ON NEURAL NETWORK AND GENETIC ALGORITHM

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ABSTRACT

Firstly, according to the given configuration and dimension of composite wing model, eight kinds of typical wing internal structure layout were designed. Through the stress analysis and comparison of the failure load and weight ratio index, the double C-beam structure has the highest structural efficiency and was selected as the wing internal structure layout scheme.

Then, the sample points were selected by Latin hypercube sampling method, and the prediction effects of seven machine learning models on the failure load and weight of composite wing were compared. The BP neural network is optimized to establish the response surface model, and the prediction accuracy can reach 93.75%

Finally, a two-level optimization method is proposed, and genetic algorithm is used to optimize the position of the composite wing beam, the thickness and the lay-up sequence of the upper and lower edge panels, leading edge and skin. The rationality of the optimization results was analyzed. The optimized results show that the failure load to weight ratio index is increased by over 146% and this method can significantly reduce the cycles of FEM analysis and achieve highly accurate response approximation results.

To construct neural-network response surfaces for composite structural optimal design, Latin hypercube sampling method is used to select the most appropriate structural analysis sample points. The constructed response surfaces are used as the objective function. Together with other conventional constraints, they form an optimization design model which can be solved by genetic algorithm. This approach is highly applicable for complex composite structural design, which can effectively guide the composite wing structure optimization problem.

Industrial applications of IGA
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ISOGEOMETRIC REISSNER-MINDLIN SHELL THEORY APPLICATION TO BUCKLING BEHAVIOR IN STIFFENED THIN-WALLED STRUCTURES

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ABSTRACT

Stiffened shell structures, such as rocket casings and aircraft fuselages, play a pivotal role in the development of aerospace engineering [1]. These thin-walled structures are susceptible to buckling when enduring axial compression, which means investigation on the buckling and post-buckling behavior of these structure is of great importance [2]. As a kind of basic structural form for aerospace vehicle bodies, the stiffened shell structures are widely used and in certain degree the hub for the whole vehicle's miscellaneous systems. This result in the situation that to improve the modeling and analysis efficiency of stiffened shell structures will greatly increase the infield capacity of design department. So this research presents a framework regarding quick modeling and buckling analysis of reinforced structures with cutouts. Utilizing Non-Uniform Rational B-Splines (NURBS), we realize a parameterized modeling approach for efficiently generating analysis-suitable models. In the analysis section, an isogeometric Reissner-Mindlin shell theory is utilized, capable of handling finite rotations and large deformations [3]. The Arc-length method is additionally used to capture the complex equilibrium paths during the buckling process. Several numerical examples emphasize the notable improvement in structural load-carrying performance achieved by reinforcing these shells. The integrated design-analysis platform demonstrated significant effectiveness and convenience, enabling engineers to make informed decisions during the design and evaluation phases of aerospace vehicle bodies.

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Mesh-free particle methods for multi-physics problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A SINGLE-LAYER WALL-BOUNDARY PARTICLE MPS METHOD FOR SIMULATING MULTIPHASE FLOWS

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ABSTRACT

A Single-layer Wall-boundary Particle Moving Particle Semi-implicit (SWP-MPS) method is proposed for multiphase flows with high density ratios and violent deformation of interface. First, a particle number density compensation (PNDC) model is developed to remove the ghost particles out of boundary thoroughly. The model is verified via static pressure simulations. Then, based on previous works, the SWP-MPS method is extended to a multiphase flow solver. Finally, the SWP-MPS method is applied to model static pressure, Rayleigh-Taylor instability, sloshing flow, and two-phase dam-break. The comparative analysis with the available experimental datum and other published numerical results proved the applicability and accuracy of the proposed SWP-MPS method for simulating multiphase flows with high density ratios and violent deformation of interface.

Architected materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

REPROGRAMMABLE METAMATERIALS THROUGH IN-SITU ACTIVATION OF SNAP-THROUGH INSTABILITY

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ABSTRACT

Snapping metamaterials are designed to deliver a function that is inherently governed by their nonlinear snapping response, which is characterized by a negative incremental stiffness. Once fabricated, though, their capacity to snap in a given mode is permanently sealed into their architecture, leaving no chances to change it in service, in cases where for example snap-through is deleterious. In this work, we present a class of reprogrammable metamaterials with snap-through capacity that can be activated and deactivated in-situ. This translates into a high versatile modus operandi where the user can - post-fabrication – choose the stress-strain response to be one among three: monotonic, monostable snapping, and bistable snapping, and then switch on the fly among them, as desired. We show how this class of reprogrammable metamaterials can broaden multifunctionality in several applications ranging from mechanical logic gates to in-situ adjustable energy absorbers.

SHAPE MORPHING OF SMART PIEZOELECTRIC COMPOSITE LAMINATES USING THERMO-ELECTRO-MECHANICAL LOADING

Tongyu Wu[*1] and Shaker Meguid*[1]

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ABSTRACT

Smart composite laminates (SCLs) consist of active piezoelectric layers bonded to or embedded in a host structure to form self adaptive systems. The importance of SCLs is evident in their potential use for shape morphing, condition health monitoring, and active vibration control. In practical applications, SCLs operate over a wide temperature range and experience large deformations. However, most existing works ignored the effect of temperature and mainly focused on small deformations, which do not reflect the real working environment of this class of laminates.
In this work, a fully coupled nonlinear finite element (FE) model is developed to investigate shape morphing of an SCL plate subject to coupled thermo-electro-mechanical disturbances. Specifically, fully coupled field equations are developed for an SCL plate in which the mechanical displacement is described in terms of the third order shear deformation hypothesis and the geometric nonlinearity in terms of von Kármán's strain-displacement relationships. The governing equations are converted into a tractable FE model. Additionally, the temperature dependent behavior of the constituents of the SCL plate is also considered in our simulations.

This work introduces two control modes (open loop control and closed loop control) to study the influence of temperature upon the morphed geometry subject to varied electro-mechanical loading. The results of our comprehensive analysis reveal a decrease in the stiffness of the SCL plate with increased temperatures. This is due to the development of thermal stresses as well as the temperature dependent material properties. As a result, SCL performs better in shape morphing at higher temperatures because the SCL plate is more flexible and responds better to the electro-mechanical coupling effects. Additionally, the shape morphing controllability of SCLs with different configurations is discussed. SCL with surface bonded piezoelectric laminates is found to have the highest shape morphing capacity and the lowest control voltage, whereas the embedded and core piezoelectric laminates are less responsive and require higher control voltages.

Data science and machine learning applications for composite materials and biomedical engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FATIGUE GROWTH OF TRANSVERSE CRACK IN HIGH MANGANESE STEEL FROGS

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ABSTRACT

Railway turnouts are critical components guiding trains during track transitions, facilitating smooth and safe changes between tracks. As one of the major structural failures of turnout frogs is fatigue cracks due to the repeated wheel-frog impact, it is essential to employ an inspection schedule that constantly monitors the crack propagation while maintaining operational efficiency. Therefore, this study aims to develop an inspection scheduling strategy specifically for railway frogs made of high-manganese steel by computationally investigating the fatigue growth of transverse cracks with various conditions. The dynamic wheel-frog impact was numerically modeled using detailed finite elements to obtain the contact pressure distribution under different train speeds and axle loads. The contact pressure was then considered as the loading in the crack growth simulation formulated in the fracture mechanics to predict the propagation of transverse cracks with varied initial locations and angles. The simulation results showed that the distance between the crack and the wheel-frog impact point was found to be the most influential factor and can result in a crack growth rate that is 12 times faster. On the contrary, although train speed and axle load can somewhat affect contact pressure distribution, their effect on the crack growth per cumulative passing tonnage is insignificant. As a result, an interval approach is proposed by considering the crack growth rate and the headway to ensure enough inspections before fatigue failure.

Catastrophic failure mechanics and numerical modelling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMPORTANCE OF APPROPRIATE CONSTITUTIVE MODEL FOR HIGH-FIDELITY SIMULATION IN GEOTECHNICAL LARGE DEFORMATION ANALYSIS

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ABSTRACT

Understanding the extremely large deformation of soil, a complex challenge in geotechnical engineering, requires advanced numerical methods due to the dynamic change in soil structure. This study presents a numerical model to analyze the responses of granular soils, akin to sand, under such conditions. A series of simulations investigate the evolution of shear bands and inner soil structure during the whole process of large deformation.

Smoothed Particle Hydrodynamics (SPH) with Finite Particle Method (FPM) interpolation is used to circumvent the computational difficulties associated with mesh distortion and improve the precision[1]. Two different constitutive models are used to highlight the impact of different constitutive models on the simulation results, namely: the critical state-based hypoplastic model, adept at capturing the pressure- and density-dependent behavior of granular soils, and the Drucker–Prager model, a staple in large deformation geotechnical simulations. An adaptive explicit stress integration scheme, termed Modified Euler automatic Substepping with Error Control (M-E-SEC) is utilized to keep the calculation accuracy of localized deformation area independent from the choice of time step[2]. Additionally, a stability correction method is introduced to suppress the breakdown problem that occurs in low-stress states. The model's effectiveness is validated by simulating passive and active earth pressure tests, followed by its application to large deformation scenarios.

Comparative analysis of these models reveals that both can simulate the soil's free-surface outline shape during deformation. However, compared to the experimental snapshots, the critical state-based hypoplastic model more accurately replicates the intricate internal structure of the soil, which is unattainable by the Drucker–Prager model. The study identifies the progression of shear bands as the primary driver of internal soil structure development and movement. It emphasizes the significance of selecting an appropriate constitutive model for high-fidelity modelling in large deformation scenarios, particularly for capturing the evolution of shear bands and internal soil structures. Furthermore, the initial relative density of the soil is also found to influence the development of these shear bands significantly and, consequently, the overall internal structure.

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Data-driven approaches for solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN ACCURATE PHYSICS-INFORMED NEURAL NETWORK ARCHITECTURE FOR DETERMINING THE HETEROGENEOUS MICROMECHANICAL ELASTIC PROPERTIES OF BIOLOGICAL MATERIALS

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ABSTRACT

The heterogeneous micromechanical properties inherent in biological materials have profound engineering and medical implications. Within the engineering community, the unique combination of material microstructure and properties has inspired innovative designs of artificial organs, soft robots, and wearable devices with desirable mechanical functionalities. Concurrently, within the medical fields, the mechanical properties of tissues play a crucial role in affecting tissue regenerative capacity, host reactions to organ implants, and cancer invasion. The significance of material mechanical properties across these diverse domains has motivated a need to better understand the underlying mechanism governing the microscopic properties of biological tissues and their associated functions, whether for improving material designs or disease diagnosis. In traditional engineering, identifying the unknown material parameters requires iterative inverse finite element analyses and optimization of the constitutive parameters until the finite element model achieves an acceptable level of mechanical response, aligning with experimental data. However, these analyses often assume material homogeneity, as uncovering the microscopic elastic properties of complex materials necessitates stress distribution, a challenging task to achieve experimentally. In the present work, we propose a novel approach to identify the distribution of elastic properties in hyperelastic materials using physics-informed neural networks (PINNs) and Fourier-feature PINNs. We explore the prediction accuracies and computational efficiency of standard PINNs and Fourier-feature PINNs across three synthetic materials, each varying in structural complexity. Further, we experiment with five distinct feedforward network types within each neural network architecture (i.e., standard PINNs and Fourier-feature PINNs). The objective of this work is to identify a top-performance, versatile network architecture capable of consistently and accurately reproducing the full-field elastic properties of complex materials, with L2 relative errors of less than 5%. The results of this work have demonstrated significant potential for advancing our understanding of micromechanical behaviors in biological materials, paving the way for future innovations in engineering and medical applications.

Lattice Boltzmann modelling and study of complex flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMPROVED PHASE-FIELD-BASED LATTICE BOLTZMANN MODEL FOR DROPLET EVAPORATION AND ITS PARALLEL ACCELERATION STRATEGY

Xiaoyu Wu[*1] and Xian Wang*[1]

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ABSTRACT

In this paper, we present an improved Allen-Cahn-based phase-field lattice Boltzmann model for heat transfer in two-phase flow with evaporation. And the vapor concentration at the liquid-vapor interface is used as the driving force for vaporization. In our improved model, four distribution functions are used to describe the velocity field, the temperature field, the vapor concentration field and the phase field, where the vapor concentration and temperature fields are coupled by the Clausius-Clapeyron correlation. We evaluate several numerical tests to verify the accuracy of the presented model, including the 1D Stefan problem and the 2D droplet evaporation problem. The results obtained by this method are in good agreement with the theoretical results. A non-zero strain rate tensor results in a non-negligible term in the constitutive equation when phase change effects are taken into account. And the effect of the corresponding viscous force term on the accuracy of the model is discussed. Since the specific heat capacitance at the gas-liquid interface varies considerably, we also consider the effect on the model of the gradient term of heat capacitance [$\nabla(\rho Cp)$] in the energy equation. Meanwhile, we investigate memory optimization and parallel acceleration techniques for the LB algorithm. The Esoteric Twist algorithm, which stores the LB distribution function for only one set of data, is introduced to compare the computational performance with the regular distribution function storage algorithm. In addition, the computational performance of AC-LBM is tested using a mixed precision approach, where a lower precision number format is used to store the distribution function and a higher precision number format is used for computation in the GPU. Based on the three floating-point data formats of double precision (FP64), single precision (FP32) and half precision (FP16), the performance of the corresponding four mixed precision is tested.

Computational methods for wind energy
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SIMULATING WIND TURBINE WAKES IN THE CONTEXT OF VARYING WIND DIRECTIONS

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ABSTRACT

A large eddy simulation (LES) framework, coupled with the blade element momentum (BEM) approach for turbine parameterization, is used to simulate wind turbine wakes in turbulent boundary layer. A tuning-free Lagrange scale-dependent dynamic model is employed for the sub-grid-scale (SGS) stress parameterization. The BEM approach utilizes inputs such as blade chord and twist angle as well as airfoil lift and drag coefficients to model the blade-induced forces. The turbulent boundary layer is characterized by an imposed inflow condition, with a specified prevailing wind direction time series. During the simulation, the wind turbine turns as the wind direction changes, and its prevailing wind direction in an instant can be a certain angle with the computational grid direction (i.e., the x direction) changing from -45 to +45 degrees. Model validation is performed through comparison with measurements of a model wind turbine wake. Preliminary results are promising and show acceptable agreement with measured data.

Machine learning and data driven based engineering computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN METHOD BASED ON THE FIRST PRINCIPLES OF ELASTICITY FOR AUTOMATICALLY MODELING OF MECHANICAL SYSTEMS

ZheTong Wu[1], Hongfei Ye[1], Hongwu Zhang[1] and Yonggang Zheng[1]*

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ABSTRACT

It is of great scientific significance and application to establish simplified mechanical models for specific geometric structures to effectively capture and analyze their deformation mechanism and avoid solving complex equations of elasticity. In recent years, a data-driven paradigm has ushered in a new era of discovery in various areas, providing a promising way for extracting laws hidden in the data and system modeling. In this work, a novel data-driven mechanical modeling method based on the first principles of elasticity is proposed to construct simplified mechanical models for structures with specific geometric characteristics from the numerical solutions of elasticity. By applying this high-precision simulation data to the unsupervised data-driven equation identification method of Seq-SVF, the governing equations could be automatically identified without providing prior knowledge of their number and left-hand terms. The sparsity of equations is ensured to balance the precision and complexity of the established models to improve their interpretability and generalization ability. By applying this method to the mechanical modeling of slender structures, homogeneous and heterogeneous beam models are discovered respectively, which are founded having the same form as the Timoshenko beam model. The expression of shear correction coefficient is distinguished under three kinds of loading conditions, which modifies the classical models. Furthermore, it is worth noting that a new expression is established corresponding to a specific loading condition, and to our best knowledge, it has never been proposed by existing works. Numerical examples show that the models established by the data-driven method are closer to the high-precision solution of elasticity than the classical models. The combination of data acquisition based on the first principles of elasticity and data-driven modeling methods reduces the reliance on human intelligence and provides a revolutionary approach to model and analyze complex mechanical systems.

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PSE (Problem Solving Environment)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A STUDY OF RELATED MODELS OF RESILIENCE IN ADOLESCENCE

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ABSTRACT

In order to deal with stress and to pursue well-being, “Resilience” always appears as a keyword of this process. This study considers “Resilience” as “the ability to adapt successfully despite difficult and threatening situations” and examines related models of it. The components of “Resilience” include “personal factors”, “ability factors”, and “environmental factors”. For each of these, the “Internal Working Model (IWM)”, “Social Skills”, and “Social Support” can be noted. “IWM” refers to “mental representation extracted based on repeated interactional experiences with the object of attachment”, and can be divided into “Stable”, “Ambivalent”, and “Avoidant”. “Social Skills” refers to “verbal and nonverbal interpersonal behaviors used to respond appropriately and effectively in interpersonal situations”. “Social Support” refers to “tangible and intangible support from various people surrounding a given individual”. The purposes of this study were to examine the direct effects of “IWM”, “Social Skills”, and “Social Support” on “Resilience” and the indirect effect of “IWM” on “Resilience” mediated by “Social Skills” and “Social Support”. The hypothesized model was that the stability of “IWM”, higher “Social Skills”, and more “Social Support” would each promote “Resilience”, and the stability of “IWM” enhances high “Social Skills”, leading to increased “Social Support” and consequently promoting “Resilience”. A questionnaire survey was administered to 189 undergraduate and graduate students using the “Mental Resilience Scale”, the “Internal Working Model Scale”, the “Adult Social Skills Self-Rating Scale”, and the “Perceived Social Support Scale for Students”. The results of the structural equation modeling showed that the path from “Stable” to “Social Skills” and “Resilience”, and the path from “Social Skills” to “Social Support” and “Resilience” was significant, but the path from “Social Support” to “Resilience” was not significant. These findings suggested that “Stable” has a direct impact on “Social Skills” and “Resilience”, and “Social Skills” has a direct impact on “Social Support” and “Resilience”. According to the results, educational interventions may be essential to promote “Resilience”. Considering that “IWM” is closely related to the nurturing environment of childhood, the acquisition of appropriate family education can foster stable “IWM”. Family education, the key to laying the foundation for developing into a person with well-being, can enhance “Social Skills”, such as handling one’s emotions appropriately and developing positive and supportive relationships with others. It also promotes “Resilience”, which means coping well with stress, and mental flexibility and adaptability.

Immersed-boundary variational methods: Theory, data structures, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HIGH-ORDER EXPLICIT RE-PARAMETERIZATION OF IMPLICIT GEOMETRIES FOR ENRICHED IMMERSED FEA

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ABSTRACT

Immersed finite element methods enable the analysis of problems involving complex interface geometry, such as those originating from CT scans or topology optimized designs, bypassing the difficult task of generating body-fitted meshes. An accurate representation of the material interface geometry within the discretized finite element problem is paramount to obtaining accurate solutions, particularly if non-linear phenomena at interfaces are considered, such as in fluid and contact solid mechanics.

In this work, we adapt a quadrature algorithm pioneered by Robert Saye [1] for use in the eXtended IsoGeometric Analysis (XIGA) framework [2]. The algorithm recasts the material interfaces implicitly defined by higher-dimensional level-set functions into the graphs of lower dimension height functions, thereby recursively reducing the dimensionality of the integrals in the weak form. This robust process recovers the implicitly defined material topology inside intersected background elements without simplifications. Hence, the algorithm is of particular interest to the types of applications mentioned above.

Modifications to the algorithm enable the generation of a higher-order triangulated foreground mesh approximating the geometry which allows for easy visualization of the interfaces. Additionally, a mesh connectivity graph is built to analyze the material layout. The XIGA framework's Heaviside enrichment strategy enriches background basis functions based on the material layout within their supports. The strategy avoids artificial coupling that may otherwise occur in the vicinity of small features.

This talk will present the modified quadrature scheme and will discuss the performance of the approach. The latter includes a comparison of the presented approach with a more common templated subdivision-based approach for a non-linear contact problem weighing the benefits from a reduced number of quadrature points and improved accuracy against the computational cost of the additional pre-processing steps required.

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Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICAL FEATURES-BASED DATA-DRIVEN MODEL FOR THERMAL AND RESIDUAL STRESS EVOLUTION PREDICTION IN COLD-SPRAY ADDITIVE MANUFACTURING

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ABSTRACT

Cold spray serves as a solid-state coating deposition technology, recently employed in additive manufacturing for individual components and restoring damaged ones. Accurate prediction and management of thermal and residual stress are pivotal in the production of additive manufacturing parts, significantly influencing the properties and performance of the final products. Finite Element (FE) analyses are conventionally used to simulate the thermal and stress dynamics during the additive manufacturing process, but the simulations are high-cost and time-consuming. The primary innovation of this study lies in the development of a physically informed, data-driven model for predicting both the thermal and residual stress fields, aiming to reduce prediction costs while maintaining a high level of accuracy. To train and test the physics-based machine learning models, Finite Element simulations of cold sprayed copper-on-aluminum were conducted. The data-driven model was validated using datasets from simulations with different path patterns and deposition layers. The results demonstrated that the prediction accuracy of both thermal and residual stress exceeded 90% when compared to the simulated outcomes.

Scientific deep learning
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEEP MACHINE LEARNING FOR COMPUTER MODELLING OF POLYMER DEGRADATION

Mingxuan Xia[*1], Ran He[1], Peter Polak[1], Baber Saleem[1] and Jingzhe Pan[1]*

[1]University of Leicester

ABSTRACT

The purpose of this study is to model the degradation process of biodegradable and polymeric vascular stents by modifying the hydrolytic degradation model using artificial neural networks (ANN). The ultimate aim is to address the threat of coronary artery disease (CAD) to public health. Common treatment for CAD with non-degradable implants has a certain probability of inflammation and intimal hyperplasia . A new biomaterial that degrades is necessary to eliminate the side effects associated with the traditional materials.

A previous computational model developed by Pan and his coworker1 predicts the molecular weight change and mass loss by considering the interplay between hydrolysis reactions and diffusion of short polymer chains during the degradation process. However, as part of the governing equations, various empirical rules such as Fickian's second law for diffusion and the source for the diffusion species are assumed. These empirical rules cannot fully capture the full complexities of the processes that underpin the polymer degradation.

This talk presents an innovative approach that replaces the empirical rules with artificial neural networks (ANN) in the governing equations. A two-step training methodology is adopted: the ANNs are firstly trained using data generated from the empirical rules and then further trained using experimental data via backpropagation. In particular, a back propagation scheme is developed for ANNs embedded inside the governing equations. The datasets incorporate degradation information which is characterized through mass loss and molecular weight for PLA50 plates and films over a 30-week period. The modelling result fits the experimental data with reasonably good accuracy, indicating the potential of replacing empirical rules with ANNs, revealing possibilities for further improving model accuracy.

1 Pan, Modelling Degradation of Bioresorbable Polymeric Medical Devices.
2 'A Comparison of Balloon-Expandable-Stent Implantation with Balloon Angioplasty in Patients with Coronary Artery Disease | NEJM'.
3 Grizzi et al., 'Hydrolytic Degradation of Devices Based on Poly(Dl-Lactic Acid) Size-Dependence'.

Microstructures of chemically complex materials and their impacts on material properties from multiscale simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STOCHASTIC CONTINUUM MODELS FOR HIGH ENTROPY ALLOYS

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ABSTRACT

High entropy alloys (HEAs) are a class of novel materials that exhibit superb engineering properties. It has been demonstrated by extensive experiments and first principles and atomistic simulations that short-range order in the atomic level randomness strongly influences the properties of HEAs. We derive stochastic continuum models for HEAs with short-range order from atomistic models. A proper continuum limit is obtained such that the mean and variance of the atomic level randomness together with the short-range order described by a characteristic length are kept in the process from the atomistic interaction model to the continuum equation. The obtained continuum model with short-range order is in the form of an Ornstein—Uhlenbeck process. This approach provides a fundamental explanation to the origin of the high strength of HEAs based on the stochastic effects on the intrinsic strength.

Model-based simulations of structural responses under extreme conditions
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SPH SIMULATIONS OF METAL DIAPHRAGM FSI VIBRATION PROBLEM USING AN IMPROVED HIGH ACCURACY CONTACT ALGORITHM

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[1]*Northwestern Polytechnical University*

ABSTRACT

The fluid-structure interaction (FSI) problem of metal diaphragms under external vibration excitation is a common issue in aerospace engineering, including complex FSI phenomena at the interface between the metal diaphragm and propellant. As a Lagrangian meshless particle method, the Smoothed Particle Hydrodynamics (SPH) method has advantages in handling FSI problems. However, the treatment of fluid-structure interfaces has always been one of the main issues affecting the accuracy of the SPH method. Therefore, an improved fluid-structure contact algorithm combining the normal flux method and repulsion force boundary method is proposed in this paper. After thorough validation using a series of benchmark cases, this algorithm is applied to simulate the metal diaphragm FSI vibration. The results demonstrate that the proposed contact algorithm achieves high-precision numerical simulation of metal diaphragm FSI vibration.

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DAMAGE INSPECTION USING HIGHER ORDER MODES CLUSTER (HOMC) GUIDED WAVES AND MACHINE LEARNING MODELS

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[1]*A*Star*

ABSTRACT

Ultrasonic guided waves (UGWs) have become a prevalent choice for long-range inspection. Recently, UGWs-based techniques have garnered increasing attention, particularly within the oil and gas industry. Conventionally, UGWs-based methods operate within the low-frequency range, generating selectively non-dispersive lower-order modes in structures. Yet, the longer wavelengths inherently limit the spatial resolution of inspection. This limitation can be addressed by employing higher operating frequencies, albeit at the expense of increased dispersion. Higher order modes cluster (HOMC) encompasses multiple higher order guided waves [1,2]. Owing to their closely matched velocities, HOMC exhibits negligible dispersion over distances spanning meters. In this study, we demonstrate the interaction between HOMC waves and surface-breaking defects of various depths in a steel plate. Firstly, dispersion curves of Lamb waves in steel plates are computed and discussed to provide insights on the generation of HOMC waves. Finite element (FE) simulations are subsequently carried out to investigate the HOMC-defect interaction. Transmission and reflection coefficients are computed from simulation results, considering different defect depths. The inherent limitations associated with utilizing these coefficients are explored and discussed. Acknowledging the constraints of conventional methods reliant on HOMC, the integration of machine learning (ML) models has been employed to augment and enrich characterization capabilities. Various ML algorithms are assessed for performance, leading to the selection of the optimal one for comparison with conventional methods. It is demonstrated that the resolution of inspection can be improved.

Quantum scientific computing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATION OF FMQA FOR HYPER-PARAMETER OPTIMIZATION AND METAMODEL-BASED OPTIMIZATION IN DEM GRANULAR FLOW SIMULATIONS

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ABSTRACT

Metamodel-based optimization is extensively applied in conjunction with numerical simulation to extract the suitable parameter combination for optimal target output in a cost-effective manner. In this approach, hyper-parameter optimization (HPO) in metamodeling and metamodel-based simulation optimization (MBSO) [1] can be considered as black-box optimization problems. In recent years, quantum annealers [2] are theoretically proven to exhibit higher computational efficiency compared to classical computers. Factorization Machines with Quantum Annealing (FMQA) [3], as a black-box optimization algorithm, has gained significant attention. Its application to these two optimization problems in the field of landslide simulation and assessment have not been fully discussed. Therefore, this study explores a FMQA framework to conduct HPO for a Gaussian Process Regression (GPR) metamodel, which is used as a low-cost approximate solver of granular flow simulations for MBSO issue sequentially. The performance of FMQA is detailed estimated in the two issues.

Discrete element method (DEM) is a conventional numerical method, taking into account the behavior of individual particles. Hence, we first conduct a series of DEM granular flow simulations to generate training data for the metamodel. GPR is then adopted to create a metamodel with the hyper-parameters optimized by FMQA. Sequentially, the metamodel is utilized as an approximate solver of the DEM simulations, coupled with the FMQA for efficient exploration of high-risk parameter settings in granular flow. The performance of FMQA on these two optimization issues is numerically evaluated in comparison with random search (RS) and Bayesian optimization (BO). In both HPO and MBSO problems, FMQA shows superiority over RS, and this superiority is more pronounced in the four-dimensional MBSO problem. The result also demonstrates that FMQA is competitive compared to the state-of-the-art BO algorithm. The value of this study is that we estimated the performance and applicability of FMQA on HPO and MBSO problems, which offers experience for the future application of quantum annealing in landslide assessment.

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Complex fluid flows in engineering: Modeling, simulation, and optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTI-TARGET/MULTI-CONDITION AERODYNAMIC CONFIGURATION OPTIMIZATION OF THE HIGH-PRESSURE CAPTURING WING BI-WING CONFIGURATION

Yao Xiao[1], Siyuan Chang[1], Kai Cui[1], Guangli Li[1] and Zhongwei Tian[1]*

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ABSTRACT

The High-pressure Capturing Wing (HCW) configuration is a promising wide-speed-range aerodynamic configuration because of its high lift-to-drag ratio at hypersonic speed[1] and high lift force at subsonic speed[2]. Based on the typical High-pressure Capturing Wing configuration, four key design parameters of the capturing wing (half-span, leading edge sweep angle, trailing edge sweep angle and assembly angle of attack) are selected as optimization variables, and the surrogate model is constructed by using uniform experimental design and Latin hypercube experimental design methods, and reasonable targets are selected to carry out multiple rounds of single-target optimization for Mach number 6, 3 and 0.3 working conditions. On this basis, a series of high-performance aerodynamic configurations were obtained by carrying out multi-point/multi-objective optimization. The results show that the lift-to-drag ratio under Mach 6 and Mach 3 and the lift force at Mach 0.3 of the wide-speed-range multi-objective optimized configuration are significantly higher than the benchmark configuration. Furthermore, the parameter sensitivity analysis and the comparative analysis of the flow field of the above series configurations were carried out, and the effect of the four key design parameters of the capturing wing on the aerodynamic performance in different speed range was discovered, among which the assembly angle of attack had the most significant effect on the aerodynamic performance in the wide-speed-range.

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PARTICLE RESPONSE TO SHEAR-INDUCED LIFT IN TWO-WAY COUPLED TURBULENT CHANNEL FLOW

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ABSTRACT

Particle-laden wall-bounded turbulent flows exist widely in both environmental research, e.g. sandstorm, and engineering applications, e.g. particle-based solar-power receivers. Two-way coupled point-particle (PP) direct numerical simulation (DNS) is employed to investigate heavy particle motions in turbulent channel flow. Focus is placed on the influence of shear-induced Saffman lift on particle motion and turbulence modulation.

The carrier phase is assumed to be air and is governed by three-dimensional compressible Navier-Stokes equations. The solid particles are assumed to be identical spheres which are 1600 times as dense as air, corresponding to a real density ratio of sand to air. The particle diameter is much smaller than the Kolmogorov scale. Therefore, the Eulerian-Lagrangian PP method is employed to track particles. The inter-particle collisions, particle rotation, and heat transfer between particles and fluid are neglected in the present study. The two-way coupling feedback source terms in momentum equation and energy equation are obtained by using the Particle-in-Cell (PIC) method. The feedback terms are simply distributed onto the nearest grid to the particle.

The effects of Saffman lift on mean stream-wise particle velocity and the fluctuating particle velocity are examined due to the importance in understanding and predicting the wall erosion caused by particles. It is shown that the mean stream-wise fluid velocity agrees well with the results of single-phase flow, which obeys the law-of-the-wall, whether the Saffman lift is present or not. However, the Saffman lift alters significantly particle velocity in the near-wall region. It turns out that the particles move faster than the fluid phase along the stream-wise direction under buffer layer. This is consistent with the experimental measurement and particle-resolved (PR)-DNS for large Stokes numbers. It proves that the particle velocities given by PP-DNS with Saffman lift is closer to the reality than those obtained by PP-DNS without Saffman lift.

A Eulerian model for particle velocity is established for wall-bounded particle-laden flow by modifying Maxey's model. Particularly, the material derivatives along fluid particles in Maxey’s model is replaced by the material derivatives along solid particles. The ensemble-averaged model is closed by gradient diffusion hypothesis and concept of Prandtl mixing length. The new model demonstrates that the Saffman lift alters the stream-wise particle velocity by changing the component in the wall-normal direction, which explains why the Saffman lift alters the profile of stream-wise particle velocity. The numerical results manifest that the new model successfully reproduces the stream-wise particle velocity with different Stokes numbers.

Theory and application of provably-robust and efficient high-order methods for high-fidelity computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PROVABLY STABLE DISCRETIZATIONS OF THE KZK EQUATIONS USING SUMMATION BY PARTS OPERATORS AND SIMULTANEOUS APPROXIMATION TERMS

Zhongyu Xie[*1], David Del Rey Fernández[1] and Sivabal Sivaloganathan[1]*

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ABSTRACT

Over the last two decades, High Intensity Focussed Ultrasound (HIFU) has emerged as a promising non-invasive medical approach for precisely ablating local tissues, offering versatile applications in tumor treatment, drug delivery, and addressing brain disorders such as essential tremor. Its advantages include targeted energy delivery with no affect on skin integrity, low system maintenance costs, minimal impact on normal tissues, and swift recovery.

Despite its' merits, HIFU remains underutilized, primarily employed in specific breast cancer and prostate cancer treatments. To expand its range of applicability, a comprehensive understanding of the interaction between the ultrasound beam and local tissues at the focal point is essential. This study focuses on modeling critical nonlinear effects in the thermal modulation of local tissues by numerically solving the Khokhlov-Zabolotskaya-Kuznetsov (KZK) equation—which is an excellent model for the nonlinear acoustic field arising in HIFU.

Constructing stable discretizations poses challenges due to polynomial nonlinear terms and a second derivative of an integral term within the KZK equations. Employing a continuous Galerkin approach, an operator is formulated to approximate the integral term, facilitating the construction of a modified second derivative operator. This establishes a clear correspondence between continuous and discrete stability proofs. Additionally, a skew-symmetric splitting technique is used to discretize the nonlinear advective term. The proposed scheme's stability under periodic boundary conditions is proven, followed by temporal advancement using a fourth-order Runge-Kutta method. The accuracy of the resulting numerical methodology is rigorously evaluated using the method of manufactured solutions.

Computational mechanics in Canada and China: Current states of shared scientific interests and opportunities for the future cooperation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STUDY ON DYNAMIC MECHANISM OF HIGH-SPEED IMPACT BETWEEN A LIQUID WEDGE AND A LIQUID SURFACE

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ABSTRACT

The impact between deformable (liquid) objects is a very fundamental problem widely existed in many highly transient multiphase flow phenomena, such as droplets impact water, bubble collapse and impact welding. Especially for the high-speed impact problem at a wedge angle, a series of complex and violent phenomena would be accompanied, including local extremely high pressure, shock wave and high-speed jet. In this work, a computational multi-component compressible flows program is employed to investigate the dynamic process of high-speed impact between a liquid wedge and a liquid surface at different wedge angles. In order to more accurately understand the properties and the generation mechanism of the high-speed jet during the impingement, the effect of surface tension is further considered. The relationships of the impact conditions with the water hammer pressure, shock waves, and the slip lines are theoretically discussed in detail. By considering the water hammer shock wave on both sides of the impact fluid, a dynamical model for the liquid wedge impact problem is established. The strength of water hammer pressure, the values of shock wave angle and slip line angle are all precisely predicted by this model compared with the numerical results. Meanwhile, the detached region of the water-hammer shock wave which is closely related to formation of the high-speed jet is also discussed.

Multi-scale, multi-rate damage and fracture: Models, experiments, and simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DAMAGE CHARACTERIZATION OF THERMAL BARRIER COATINGS UNDER CMAS CORROSION

Kun Xiong[*1], Ziyang Zhou[1], Jingjing Yang[1] and Xueling Fan[1]*

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ABSTRACT

The silicate particles, such as volcanic ash, dust and sand, impact the turbine blade with high temperature and high-speed gas and deposit on the surface of the thermal barrier coating. The molten CMAS penetrates into the coating and causes cracks in the coating, resulting in peeling failure of the coating, which has become one of the main reasons for the failure of thermal barrier coatings (TBCs) system. In this paper, the failure behavior of EB-PVD thermal barrier coatings under CMAS corrosion was studied. The critical failure strain of the surface of TBCs under different corrosion time was obtained, and the failure criterion of TBCs under CMAS corrosion was established. The results show that the infiltrated CMAS not only changes the mechanical properties of the penetration zone, but also reacts with the coating. The reaction between CMAS and thermal growth oxide (TGO) layer destroys the TGO, causing the delamination of the TBCs at the interface. Based on the buckling theory, the damage model of TBCs was established, and the relationship between the interface damage and the surface strain of TBCs was obtained. With the increase of corrosion time, the damage of TBCs accumulated continuously and showed a similar parabolic trend. When the damage accumulated to the critical value, the coating spalling failure occurred. The results provide a theoretical basis for the damage quantification and evaluation method of TBCs under CMAS corrosion conditions.

DATA DRIVEN MODELING OF UNKNOWN STOCHASTIC DYNAMICAL SYSTEM

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ABSTRACT

We discuss a general framework for data driven modeling of unknown stochastic differential equations (SDEs). Given short bursts of trajectory data, our method is able to construct an accurate numerical model for the underlying (and unknown) SDEs. The method utilizes flow map learning (FML) technique that was developed for modeling deterministic systems. For modeling SDEs, our method employs generative models to accurately approximate the one-time-step conditional probability distribution of the system. Under the framework, generative models such as GANs, normalizing flow, diffusion model can be employed. Using an extensive set of examples, we demonstrate that the method is highly versatile, robust, and can provide accurate system predictions for very long time domain far exceeding that of the training data. The learned numerical models can also capture small probability system transitions that are not observed in the training data.

THREE-DIMENSIONAL STABILIZATION-FREE VIRTUAL ELEMENT METHOD FOR NONLINEAR PROBLEMS

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ABSTRACT

The Virtual Element Method (VEM) can be regarded as a generalization of the classical finite element method (FEM) to general polygonal meshes. In the prior studies of the VEM, a stabilization term is required in order to ensure that the global stiffness matrix has the correct rank. In this work, we present a stabilization-free Virtual Element Method for hyperelastic materials in 3D. The main idea of the stabilization-free approach is to use an enhanced approximation space to compute a higher-order polynomial L2 projection of the gradient. This work describes the calculation process of the origibal H1 projection operator and the highrt-order L2 projection operator for three-dimensional problems. The formulation of the stabilization-free VEM for 3D hyper-elastic materials is given in the next. Some numerical examples are given to compare the accuracy of the stabilization-free VEM with the conventional VEM.

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Physical models and reduced order models augmentation with data for physics-informed machine learning in real-world applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MULTI-FIDELITY DEEP OPERATOR NETWORK (DEEPONET) FOR FUSING SIMULATION AND MONITORING DATA: APPLICATION TO REAL-TIME SETTLEMENT PREDICTION DURING TUNNEL CONSTRUCTION

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ABSTRACT

The assessment of surface settlements during mechanized tunneling is of importance and remains a challenging research topic. Generally, the surface settlement can be predicted using different paradigms: either a physics-driven approach utilizing computational models, or a data-driven approach employing machine learning techniques to establish mappings between influencing factors and ground settlement. In this work, we introduce a multi-fidelity deep operator network (DeepONet) framework to combine the advantages of both approaches and assimilate the data from different sources. The presented framework, which leverages the recently developed operator learning methods, comprises two components: a low-fidelity subnet that captures the fundamental ground settlement patterns obtained from finite element simulations, and a high-fidelity subnet that learns the nonlinear correlation between numerical models and real engineering monitoring data. The results show that the proposed method can capture not only the physical laws governed by numerical simulations, but also accurately fit measured data as well. Remarkably, even with limited noisy measurement data, our model can still provide rapid, precise, and robust reconstruction of the full-field surface settlement in real-time during mechanized tunneling.

Computational fluid dynamics (CFD) and fluid-structure interaction (CFSI): Methods and Applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A (WEIGHTED) SHIFTED BOUNDARY METHOD FOR MOVING BOUNDARY PROBLEMS

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ABSTRACT

The Shifted Boundary Method (SBM) belongs to the class of unfitted (or immersed or embedded) finite element methods and was recently introduced for the Poisson, linear advection/diffusion, Stokes, Navier-Stokes equations, and many additional problems. By reformulating the original boundary value problem over a surrogate (approximate) computational domain, the SBM avoids integration over cut cells and the associated problematic issues regarding numerical stability and matrix conditioning. Accuracy is maintained by modifying the original boundary conditions using Taylor expansions. Hence the name of the method, that shifts the location and values of the boundary conditions. In the context of applying the SBM to incompressible flows involving moving boundaries or free surfaces, spurious pressure oscillations in time may result from a discrete change of the total volume of active fluid over a time step. To avoid this issue, a weighted SBM is proposed, in which the variational form of the equations is weighted by the elemental volume fraction of active fluid. The proposed weighted SBM (or W-SBM) exactly preserves states of hydrostatic equilibrium, and induces small mass (i.e., volume) and momentum conservation errors, which converge as the grid is refined. This is in analogy to cutFEMs and related unfitted approaches, which rely on an affine representation of cut boundaries. We demonstrate the robustness and accuracy of the proposed method with an extensive suite of two-dimensional and three-dimensional tests for incompressible Stokes and Navier-Stokes Flows.

Battery modeling and computation: From material to device
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

QUANTITATIVE ANALYSIS OF ELECTROCHEMICAL-MECHANICAL COUPLING BEHAVIORS IN LITHIUM-ION BATTERIES

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ABSTRACT

The safety and durability of Lithium-ion batteries (LIBs) are intrinsically interconnected phenomena, intricately woven with electro-chemo-mechanical dynamics. A comprehensive comprehension of these multifaceted interactions necessitates interdisciplinary endeavors. In this study, we meticulously formulate and execute mechanically constrained charging/discharging characterizations, employing a collaborative approach that integrates multiphysics modeling. This holistic methodology aims to elucidate the intricate coupling mechanisms inherent in the solid-liquid electrode-electrolyte interface and the interaction between solid-solid active materials within LIBs.

Our investigations reveal that a LIB cell subjected to mechanical constraints manifests an elevated voltage profile during charging and a reduced charging duration. This phenomenon can be attributed to augmented electrolyte resistance and diminished diffusivity resulting from a concurrent decrease in electrode porosity. The observed reaction force response of the cell is a confluence of the mechanical response of the cell structure and the electrochemical volume variations induced by Li-ion intercalation/de-intercalation processes. Notably, under mechanical constraints, the cell's capacity experiences a significant reduction in scenarios involving fast-charging; however, employing a constant-voltage charging protocol facilitates a noteworthy capacity recovery.

This study underscores the potential of multiphysics approaches in unraveling the electrochemical-mechanical coupling mechanisms, thereby providing valuable insights for directing battery system design and management strategies. The results presented herein offer a promising trajectory for advancing our understanding of LIBs and optimizing their performance through informed and targeted design interventions.

Numerical modelling of composite materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTI-SCALE MODELING FOR TENSILE BEHAVIOR OF PLAIN WOVEN SIC/SIC COMPOSITES CONSIDERING TEMPERATURE AND OXIDATION

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ABSTRACT

Ceramic matrix composites (CMCs) have a broad application prospect in high-performance aero-engine because of its excellent high-temperature comprehensive mechanical properties. The mechanical behavior and performance prediction of CMCs can provide theoretical basis and engineering methods for material design, structural analysis, and machining forming. In this paper, the tensile damage and fracture process of fiber-reinforced SiC/SiC CMCs under high temperatures and oxidizing atmosphere were investigated, then the damage mechanisms of the interface oxidation and the fiber thermal failure were considered in the stress distribution, matrix multi-cracking, interface debonding and material failure analysis. A first matrix cracking stress model and a constitutive model of unidirectional SiC/SiC CMCs were developed. The key damage variables were transferred to the fiber bundle material parameters in plain woven SiC/SiC CMCs finite element model based on real structure. Finally, a multi-scale constitutive model considering temperature and oxidation was established. Using this constitutive model, a numerical modeling for tensile behavior of plain woven SiC/SiC CMCs at different oxidation times (0-2 hours) and temperatures (25-1200℃) was conducted. The stress-strain response of plain woven SiC/SiC CMCs exhibits significant temperature and oxidation time correlations. The initial elastic modulus of CMCs remains unchanged with increasing oxidation time at the same temperature, while the tensile strength decreases with increasing oxidation time. The established multi-scale model can reasonably predict the tensile behavior and performance degradation, and the simulation curve is consistent with the experimental values.

Keywords: Ceramic matrix composites; Multi-scale modeling; Tensile behavior; Thermal stress; Oxidation

New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BUCKLING TOPOLOGY OPTIMIZATION USING A LINEAR MATERIAL MODEL

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ABSTRACT

In recent decades, topology optimization has been increasingly used in structural design due to its capacity to generate efficient structures with minimal materials. Given the prevalence of compressed slender members in such optimized structures, buckling emerges as a critical factor in topology optimization. A major challenge in the buckling topology optimization of continuum structures is addressing pseudo buckling modes in intermediate and low-density elements. These modes arise from penalized material interpolation schemes and the presence of stress singularities. This study tackles the issue by employing a linear material model for both stiffness and stress stiffness matrices, combined with ε-relaxation functions to effectively mitigate pseudo buckling modes. The presented algorithm is established based on the floating projection topology optimization (FPTO) method. Owing to the effective elimination of pseudo buckling modes, the optimization process achieves great stability and can be conducted from the full design domain. Numerical results demonstrate a uniform strain energy density distribution across the optimized structures, highlighting the effectiveness and efficiency of the proposed algorithm. Furthermore, the smooth and practical designs obtained through the FPTO method are readily applicable to fabrication processes, marking a significant advancement in the field of structural topology optimization.

Phase-field models of fracture
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RATE-DEPENDENT PHASE-FIELD COHESIVE THEORY: A UNIFIED MODEL FOR DYNAMIC CRACK BRANCHING VIA ESHELBY ENERGY-FLUX INTEGRAL

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ABSTRACT

As the crack propagation achieves a critical velocity, the stability of dynamic front sharply decreases and even begins branching. Such critical velocity is controlled by the velocity/rate dependent fracture energy. To address the toughening process, the phase-field fracture model considering variational consistency converges to a rate-dependent cohesive zone model, where the viscous resistance is proposed without ad hoc assumption. In the crack front dynamics, the fundamental understanding of the toughening zone shape and size is still lacking, and the specific contribution of cohesiveness and viscosity to the total dissipation is still unclear. In this work, the 1-D tensile bar model has been obtained for detecting the material constitutive response (i.e., traction-separation law), where the phase-field model (PFM) is controlled by a parabolic PDE with nonlinear boundary conditions and source terms. The intrinsic separation law of the phase-field constitutive property is discovered (similar to the elasto-viscoplasticity). Meanwhile, based on the equilibrium of the Eshelby energy-flux integral around the phase-field crack tip, the compatibility conditions of the three intrinsic parameters (degradation, geometric, and viscosity coefficients) are verified during the dynamic crack branching. The proposed PFM matches well with the dynamic fracture energy and critical velocity of branching among the various materials (Soda-lime glass, PMMA, Homalite-100, and Steel) in a unified framework, where the toughening behavior is governed by a normalized toughening coefficient (F_V=c_R⁄(G_C*M)). The scaling analysis of the dissipative mechanism around the crack tip demonstrates that the remarkable viscous dissipation occurs among preexisting cohesive zone, driven by the ultra-high strain rate, and the dissipative mode transition follows a universal master curve among the dimensionless inertance, cohesiveness, and viscosity parameters.

Inverse and optimization problems for advanced materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INVERSE DESIGN OF SEISMIC METAMATERIALS BASED ON MACHINE LEARNING

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ABSTRACT

The ability to efficiently design seismic metamaterials with desired functional characteristics on-demand represents the next frontier in metamaterials discovery. However, traditional gradient and non-gradient-based optimization algorithms still face difficulties in convergence and high computational cost when dealing with increasing optimization parameters. To address the inherent challenges of traditional inverse design methods, this study employs deep learning to design seismic metamaterials with specific band gaps. Firstly, a machine learning-based surrogate model is constructed to rapidly generate a dataset of three-dimensional seismic metamaterial features and their associated band structures. Subsequently, this dataset is utilized to train the inverse design deep network. Numerical experiments demonstrate that the proposed optimization strategy can efficiently design seismic metamaterials with the demanded band gap.

Keywords: Inverse design, seismic metamaterial, surrogate model, deep learning

Numerical modelling of composite materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFECTS OF MATERIAL PROPERTY UNCERTAINTY ON FRACTURE MODELING OF UNIDIRECTIONAL DOUBLE CANTILEVER BEAM SPECIMENS

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ABSTRACT

Some composite materials exhibit spatially varying material properties stemming from the inherent randomness in their microstructures. The variation in material properties potentially results in uncontrollable random fracture initiation, which should be considered in preliminary design studies. Among all the fracture modes, composite materials primarily experience fracture through the opening mode (Mode-I), and the Mode-I cracks could alter the local stress states to initiate other fracture modes. This study focuses on the implementation of stochastic material inputs into the double cantilever beam (DCB) analysis for unidirectional (UD) composite laminates. A parametric study of Abaqus finite element (FE) models are conducted to observe how Mode-I fracture is influenced with and without stochastic material properties in the DCB models. A Box-Mueller algorithm [1] is implemented by a user-defined subroutine to generate random composite ply and cohesive properties with random variations ranging from 5% to 30% of mean values. These stochastic material inputs are also randomly assigned to individual finite elements. The results reveal that increasing variations in input properties for both cohesive elements and composite lamina elements leads to a large failure envelope, with the stochasticity of the cohesive elements having a greater impact on failure than that of the lamina elements. These findings demonstrate the need to account for spatially varying properties in composite fracture models to avoid overpredicting actual strength in composites with inherent randomness. It is important to note that conventional composite fracture models are predominantly within a deterministic framework and these models often overpredict fracture performance [1,2]. The stochastic failure model in this study can be easily applied in composite analysis with inherent material variations or uncertainties such as short fibre composites. This makes the technique broadly relevant for prognostic health monitoring (PHM) and a progressive damage model incorporating material property uncertainties.

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New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE INFLUENCE OF DENSITY INTERPOLATION FUNCTION IN DYNAMIC TOPOLOGY OPTIMIZATION

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ABSTRACT

In the realm of topology optimization, the interpolation function that transforms binary integer problems into continuous problems has always been a critical component. This encompasses interpolation functions for Young's modulus and density. Conventional methods such as the SIMP method and RAMP method typically introduce penalty factors only in the Young's modulus interpolation function to facilitate the convergence of optimization algorithms, while employing linear interpolation for density. This approach is effective in static topology optimization, where the motion equation Ku=F is independent of mass. However, in dynamic topology optimization, the form of the motion equation becomes Ma+Ku=F, the dynamic influence of density on the system must be considered. Therefore, continuing to use linear interpolation functions on density may lead to a range of issues, including grayscale problems and structurally unreasonable outcomes.

To address this challenge, the present study thoroughly examines the influence of various density interpolation functions on optimization results. Considering multiple influencing factors, including the ratio of Young's modulus to density, the magnitude of applied loads, and the frequency of loads, we conduct a detailed analysis of how these factors affect the optimal density interpolation in the context of dynamic topology optimization. The objective of this research is to enhance the accuracy of the optimization model, ensuring structural robustness and excellent performance in dynamic problems.

Through systematic investigation, the present study unveils the significance of selecting appropriate density interpolation functions in dynamic topology optimization. The collaboration between different density interpolation functions and Young's modulus interpolation functions significantly influences the results of dynamic topology optimization for structures. This not only contributes to a better understanding of structural behavior under diverse conditions but also offers novel perspectives and approaches for the design and optimization of future engineering structures.

In summary, this research provides valuable insights for the further improvement of dynamic topology optimization methods. These insights are poised to drive the broader adoption of topology optimization methods in practical engineering applications, thereby offering more effective tools and guidance for structural design and performance optimization.

Advances in multi-scale, multi-material, and multi-component Topology Optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE TOPOLOGY OPTIMIZATION FOR CFRP STRUCTURES WITH ADDITIVE MANUFACTURING

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ABSTRACT

Additive manufacturing (AM) is attracting widespread interest as an effective tool to fabricate sophisticated structural components for a range of industrial applications such as aerospace, automotive, biomedical, construction, etc. Compared with conventional manufacturing technologies, AM allows accommodating various complex topological designs and minimizing material waste and lowering the costs of molds or tools. Concerning composite materials, AM provides more potential and flexibility to improve structural performances by creating sophisticated product designs with better use of material constituents [1]. More specifically, combining topology optimization and additive manufacturing (AM) enables the full exploitation of the capacity for heightening the performance of carbon fibre reinforced plastic (CFRP) structures. This study simultaneously performs topology optimization and fibre path design by employing the radial basis function (RBF) based level set function (LSF) [2]. Fiber paths are determined instinctively for the inherent advantages of the LSF, and fibre orientations are parameterized accordingly. Manufacturing drawbacks such as gaps and overlaps can be avoided by introducing a fast-marching method [1]. To verify the effectiveness of the optimization method, three groups of optimized and empirical designs are fabricated by the AM technique, respectively, and the experimental tests are further carried out. Finite element (FE) models are also reconstructed for the 3D printed structures, and then the FE simulation is validated by the experimental tests. With the proposed optimization method, stiffnesses for all three groups of the optimal samples are significantly improved compared with the empirical counterparts. The FE modeling technique is capable of replicating the experimental results [1]. This study paves a new way to develop an integrated framework of optimization, additive manufacturing, experimentation, and validation to deliver high-performance CFRP structures.

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Uncertainty quantification and reliability analysis in engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MESOSCOPIC DOMAIN DECOMPOSITION APPROACH COMPOSED WITH PRECONDITIONED CONJUGATE GRADIENT FOR MODELING CONCRETE

Yang Xu[*1] and Zhang Lin*[1]

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ABSTRACT

The mesoscopic numerical method is a powerful tool for simulating concrete's mechanical behavior. However, most mesoscopic finite element methods (FEM) would consume a lot of computing resources according to the considerable elements, which is especially marked when analyzing models with a larger size. To provide a comprehensive and efficient simulator to predict the concrete's mechanical behavior, a mesoscopic domain decomposition (MDD) approach technique composed of the Preconditioned Conjugate Gradient (PCG) method is employed in this study. A group of meso-models of concrete, which were considered as a three-phase composite, consisting of aggregates, cement paste, and the interface transition zone between them. Then, these models were analyzed by the FEM and the MDD approach technique composed with PCG, respectively. By comparing with the experimental benchmark, the simulation results were validated. The computation demonstrated that the MDD approach technique composed with PCG would cost less computing time, which could provide a reasonable tool for understanding and predicting the observed macroscopic behavior of concrete.

Keywords: concurrent multiscale, finite element method, domain decomposition, Preconditioned Conjugate Gradient

Quantum scientific computing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

QUANTUM COMPUTING ENHANCED DISTANCE-MINIMIZING DATA-DRIVEN COMPUTATIONAL MECHANICS

Yongchun Xu[*1], Zengtao Kuang[1], Jie Yang[1], Qun Huang[1], Wei Huang[1] and Heng Hu[1]*

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ABSTRACT

Data-driven computational mechanics [1] has great potential in engineering applications by eliminating material modeling errors and uncertainty. In this computational framework, the solution-seeking procedure relies on minimizing the distance between the constitutive database and the conservation law. However, it currently suffers from computational efficiency issues in data search, especially when dealing with large-scale databases. Specifically, assume that a data search is conducted in a database with N data, and the dimension of data is D. In one nearest neighbor search, the computational complexity on a classical computer requires executing N distance calculations, each with a cost of O(D), resulting in the total computational complexity O(ND).

Addressing this challenge, we have introduced a novel framework named quantum computing enhanced data-driven computational mechanics (qDD) [2]. Our method employs an efficient quantum algorithm to estimate the distance between two data, which exponentially reduces the computational complexity from O(D) to O(log D), thus reducing the overall complexity to O(N log D). The proposed method is not only validated on the quantum computer simulator Qiskit, but also on a superconducting quantum computer from Origin Quantum.

Furthermore, quantum hardware noise remains a critical barrier to achieving accurate simulation results due to the limitation of the current Noisy Intermediate-Scale Quantum (NISQ) hardware level. We have used an error mitigation technique, zero-noise extrapolation (ZNE), to improve the accuracy of qDD when operating on a noisy quantum computer [3]. A data-driven multiscale simulation of a composite L-shaped beam confirms the effectiveness of the proposed approach. We believe the introduction of qDD represents a promising step towards using the power of quantum computing in computational mechanics and explores a new computational paradigm for further advancements in the field.

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Advance modeling and simulation in complex porous media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A THEORY OF HYDROGEL MECHANICS THAT COUPLES SWELLING AND EXTERNAL FLOW

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ABSTRACT

Two aspects of hydrogel mechanics have been studied separately in the past. The first is the swelling and deswelling of gels in a quiescent bath of solvent, and the second is the solvent flow around and into a gel domain. The former neglects convection driven by external flow, whereas the latter neglects solvent diffusion driven by a gradient in chemical potential. Motivated by engineering and biomedical applications where both aspects coexist and potentially interact with each other, this work presents a poroelasticity model that integrates these two aspects into a single framework and demonstrates how the coupling between the two gives rise to novel physics in relatively simple one-dimensional and two-dimensional flows.

Recent advances on interfaces dynamics modeling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ENERGETIC VARIATIONAL NEURAL NETWORK DISCRETIZATIONS OF GRADIENT FLOWS

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ABSTRACT

In this talk, I will describe structure-preserving neural-network-based numerical schemes to solve both L2-gradient flows and generalized diffusions. By using neural networks as tools for spatial discretization, we introduce a structure-preserving Eulerian algorithm to solve L2-gradient flows and a structure-preserving Lagrangian algorithm to solve generalized diffusions. The Lagrangian algorithm for a generalized diffusion evolves the “flow map" which determines the dynamics of the system. This avoids the non-trivial task of computing the Wasserstein distance between two probability functions. Unlike most existing methods that construct numerical discretizations based on the strong or weak form of the underlying PDE, our schemes are constructed using variational formulations of these PDEs for preserving their variational structures. Instead of directly solving the obtained nonlinear systems after temporal and spatial discretization, the minimizing movement scheme is utilized to evolve the solutions. This guarantees the monotonic decay of the energy of the system, and is crucial for the long-term stability of numerical computation. I will describe a few numerical experiments to demonstrate the accuracy and energy stability of the numerical schemes. This is a joint work with Profs. Yiwei Wang and Chun Liu.

Uncertainty quantification and scientific machine learning for predictive modeling of complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DNN MODELING OF UNKNOWN PDE SYSTEMS

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ABSTRACT

We discuss a data driven modeling framework called Flow Map Learning (FML) for modeling unknown PDE systems. Unlike other system discovery methods that seek to discover the governing equations, our method construct an accurate numerical approximation to the flow map operator of the unknown system. For PDE systems, a specialized DNN structure is required to enforce the learning of the various differential operators in the system. The method can also model PDE systems when only partial data are available. Using an extensive set of examples, we demonstrate the efficacy and robustness of the method to a variety of PDEs, as well as nonlocal problems involving fractional PDE.

Uncertainty quantification and reliability analysis in engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN ACTIVE LEARNING KRIGING METHOD BASED ON SPHERICAL DECOMPOSITION-MCS (AK-SDMCS) FOR STRUCTURAL RELIABILITY ANALYSIS WITH SMALL FAILURE PROBABILITIES

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ABSTRACT

The main challenge in structural reliability analysis is accurately estimating the failure probability while minimizing number of calls to the performance function. However, evaluating the performance function has significant computational costs. To enhance computational efficiency, easily computed metamodels are often utilized to substitute the performance function. Specifically, active learning reliability methods combining adaptive Kriging and simulation methods like AK-MCS (an active learning method combining adaptive Kriging and Monte Carlo Simulations) [1], which integrate the benefits of high computational efficiency of metamodels and high accuracy of simulation methods, have gained substantial attention in recent years.

Nevertheless, AK-MCS can be computationally demanding for small failure probabilities due to repeated runs of Kriging on a candidate pool with a large number of samples. To address this challenge, this paper proposes a novel active learning reliability method, termed AK-SDMCS, combining adaptive Kriging and spherical decomposition-MCS. The fundamental concept involves dividing the sample population of AK-MCS into non-overlapping subsets using a strategic spherical decomposition of the parameter space. Subsequently, Kriging is updated layer by layer through active learning while following the process of space decomposition. This approach allows for efficient active learning of Kriging, as the number of samples in the decomposed spherical rings is significantly smaller than in AK-MCS. Additionally, the number of samples in the spherical rings can be flexibly allocated based on the associated estimator variance, and hence reducing the total number of candidate samples. Furthermore, certain modifications have been implemented to enhance the computational efficiency of active learning.

Given the efficiency of active learning and the fast evaluation capability of the Kriging metamodel, the proposed AK-SDMCS method offers an implementable, accurate, and efficient option for analyzing reliability in scenarios with small failure probabilities. Moreover, AK-SDMCS maintains the generality of MCS. Three academic examples are presented to validate the effectiveness and efficiency of the proposed method.

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Methods for identification, machine learning, and uncertainty quantification of reduced order models of coupled systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADVANCEMENTS IN GS4-I-ROM: A UNIFIED TIME INTEGRATION FOR COUPLED FIRST-SECOND ORDER TIME-DEPENDENT PROBLEMS

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ABSTRACT

Over the years, there has been significant progress in the development of time integration algorithms for solving time-dependent problems in computational mechanics. These algorithms play a crucial role in solving first-order transient systems (e.g., fluid dynamics, heat transfer) or second-order transient systems (e.g., structural dynamics, wave propagation). Notable examples of these algorithms include LMS, composite method, and time finite element method. In previous research, Tamma's group introduced the Generalized Single-Step Single-Solve Isochronous time integration (GSSSS i-integration) approach. This innovative method allows for the direct solution of both first-order and second-order transient systems, as well as their coupled systems, without relying on separate frameworks [1]. The GSSSS i-integration is based on a three-root system that utilizes the u-v-a set of variables to adapt the two-root system (u-v system), resulting in the inclusion of a dummy variable in the scheme.
This study presents an alternative perspective on the GSSSS i-integration that starts from the u-v system and naturally extends to cover the u-v-a systems. By adopting this approach, all physics fields in both first- and second-order systems are naturally incorporated without the need for dummy variables. We demonstrate that desirable numerical features such as energy conservation, controllable numerical dissipation, second-order accuracy, and zero-order overshoot can be achieved by tuning only two algorithmic parameters. Furthermore, we integrate the proposed isochronous schemes with the proper orthogonal decomposition (POD) technique to create a unified model order reduction framework called GS4-i-ROM. This framework enables the solution of coupled problems under a single analysis, incorporating the most comprehensive set of optimal and compatible algorithms. To illustrate the effectiveness of our approach, we apply it to classical one-way and two-way coupled thermoelastic problems[2]. Through these examples, we demonstrate the adaptive procedure and numerical performance of the GS4-i-ROM approach, highlighting its improved efficiency in solving coupled problems. Ultimately, we aim to implement the GS4-i-ROM approach in studying structure/thermal/fluid interactions within computational mechanics, thereby enhancing the accuracy, efficiency, and robustness of numerical simulations involving coupled physics.

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Data-driven approaches for solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREDICTING LINEAR AND NONLINEAR STRESS DISTRIBUTION IN COMPOSITES USING INTEGRATED CONVOLUTIONAL AND GRAPH NEURAL NETWORKS

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ABSTRACT

This work introduces CompINet, a novel deep learning (DL) method to predict the linear and nonlinear stress fields in composites with high accuracy. Predicting the stress distribution in structures subjected to external loads is a crucial step in evaluating damage initiation and propagation, which are key components for structural design and optimization. While Finite Element Method (FEM) is commonly used for stress analysis, it becomes computationally expensive for complex geometries and nonlinear problems like composite materials. Thus, this study aims to propose a fast and accurate surrogate for FEM using deep learning.

Our proposed framework, CompINet, integrates graph neural network (GNN) and convolutional neural network (CNN) to predict both linear and nonlinear von-Mises stress distributions within the microstructural representation of fiber-reinforced composites. CompINet is inspired from the similarity between fiber-reinforced composite microstructures, especially the spatial arrangement of fibers and the distances between them, alongside the concept of graph neural networks. GNN is adept at capturing interactions and relationships between individual fibers, while CNN excels at extracting pixel-wise features. This combination offers a comprehensive analysis of the stress field. Moreover, particular emphasis is placed on predicting the stress distribution at the fiber/matrix interface, where a high error concentration is observed. This challenge has been addressed by incorporating a targeted physically-based method to further improve the stress field prediction. To generate the required data set, a nonlinear cohesive interface-enriched generalized finite element method (IGFEM) framework is used to simulate the microstructural representations of a fiber-reinforced composite. We assume that the fibers are linearly elastic, whereas the matrix has an elastic-plastic behavior, and we use a continuum damage relationship to predict the initiation and evolution of matrix damage. A cohesive zone model is used to simulate the interfaces. CompINet demonstrates exceptional performance and accuracy, achieving better results compared to existing DL frameworks despite using a training and validation dataset 20 times smaller. Trained with only 250 samples, CompINet achieves a mean R2 value of 0.96, emphasizing its exceptional predictive capabilities.

Quantifying epistemic uncertainties for computational predictions
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STOCHASTIC SUBSPACE VIA PROBABILISTIC PRINCIPAL COMPONENT ANALYSIS FOR MODEL-FORM UNCERTAINTY

Akash Yadav[*1] and Ruda Zhang*[1]

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ABSTRACT

This paper proposes a probabilistic model of orthonormal matrices based on the probabilistic principal component analysis (PCA). Given a sample of vectors in the embedding space, commonly known as a snapshot matrix, this method uses quantities derived from the PCA to construct distributions of the sample matrix as well as orthonormal matrices of all ranks. It is applicable to projection-based reduced-order modeling methods, such as proper orthogonal decomposition and related model reduction methods. Whereas existing methods use tangent space of a matrix manifold to carry out probabilistic modeling of reduced-order basis, the proposed method carries out the probabilistic modeling of the subspace itself. This approach helps us find the probability distribution's analytical form in certain cases. The stochastic reduced order basis (SROB) thus constructed can be used, for example, to characterize epistemic uncertainity and model-form uncertainty in particular in computational mechanics. The proposed method has multiple desirable properties: (1) it is naturally justified by a probabilistic interpretation of PCA and has analytic forms for the induced probabilistic models on related matrix manifolds; (2) it satisfies linear constraints, such as boundary conditions of all kinds, by default; (3) it has only one hyper-parameter, which greatly simplifies hyper-parameter training; (4) its algorithm is very easy to implement. We compare the proposed method with existing approaches visually in a low-dimensional example and demonstrate its performance in characterizing the uncertainty in a dynamics model of a space structure.

UQ-TTA student paper competition in uncertainty quantification
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STOCHASTIC SUBSPACE VIA PROBABILISTIC PRINCIPAL COMPONENT ANALYSIS FOR MODEL-FORM UNCERTAINTY

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This paper proposes a probabilistic model of orthonormal matrices based on the probabilistic principal component analysis (PCA). Given a sample of vectors in the embedding space, commonly known as a snapshot matrix, this method uses quantities derived from the PCA to construct distributions of the sample matrix as well as orthonormal matrices of all ranks. It is applicable to projection-based reduced-order modeling methods, such as proper orthogonal decomposition and related model reduction methods. Whereas existing methods use tangent space of a matrix manifold to carry out probabilistic modeling of reduced-order basis, the proposed method carries out the probabilistic modeling of the subspace itself. This approach helps us find the probability distribution's analytical form in certain cases. The stochastic reduced order basis (SROB) thus constructed can be used, for example, to characterize epistemic uncertainity and model-form uncertainty in particular in computational mechanics. The proposed method has multiple desirable properties: (1) it is naturally justified by a probabilistic interpretation of PCA and has analytic forms for the induced probabilistic models on related matrix manifolds; (2) it satisfies linear constraints, such as boundary conditions of all kinds, by default; (3) it has only one hyper-parameter, which greatly simplifies hyper-parameter training; (4) its algorithm is very easy to implement. We compare the proposed method with existing approaches visually in a low-dimensional example and demonstrate its performance in characterizing the uncertainty in a dynamics model of a space structure.

Multiphysics and data-driven modeling for cardiovascular biomedicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN EFFICIENT BEAM-TO-SHELL CONTACT FORMULATION FOR STENT DEPLOYMENT IN DEFORMABLE VESSELS

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ABSTRACT

Stent implantation has rapidly become one of the most widely adopted endovascular treatment procedures for numerous peripheral and cerebrovascular diseases. A stent refers to a small cylindrical metallic or polymer tube, that is inserted into the blood vessel via a catheter and is subsequently expanded to prop the diseased vessel open and restore blood flow. As the vessel is distended, the contact of stent with vascular wall can create non-physiological stresses. Further, given the large displacements and geometrical nonlinearities associated with stent expansion process, the final configuration of the stent within the vessel is typically not known a priori, and can lead to lengthy interventional times and complications. Therefore, there is an immediate need to develop computational algorithms that can enable virtual planning of stent deployment.

This work proposes an efficient beam-to-shell contact framework by leveraging our previous formulations for vascular wall modelling and beam-to-surface contact mechanics [1,2]. Specifically, we recently reported a nonlinear rotation-free shell formulation that utilizes only displacement degrees of freedom to calculate both the membrane and bending mode deformations of vessel wall, while also allowing us to incorporate biologically representative nonlinear constitutive models. Additionally, we have recently reported a 3D corotational formulation to simulate a beam-to-rigid surface contact. In contrast to Total Lagrangian beam formulations, this approach separates the total motion into a rigid body component and a small local deformation, resulting in a computationally efficient formulation. In the current work, we propose to simulate stent deployment in deformable vessels by developing a fully implicit algorithm to couple the contact between the rotation-free shell element and the corotational beam element. This approach represents an efficient formulation to model stent deployment in vascular vessel as, firstly, the vessel wall is represented only via mid-plane displacement degrees of freedom and, secondly, the stent is modelled using an efficient corotational formulation. The implementation of the proposed formulation is carried out within Julia as part of our ongoing open-source developments for structural biomechanics. Following the presentation of details of the formulation and implementation, we will present several examples to illustrate the efficacy and robustness of the proposed algorithm.

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Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SPDE-NET: NEURAL NETWORK BASED PREDICTION OF STABILIZATION PARAMETER FOR SUPG TECHNIQUE

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ABSTRACT

We propose SPDE-Net, an artificial neural network (ANN) to predict the stabilization parameter for the streamline upwind/Petrov-Galerkin (SUPG) stabilization technique for solving singularly perturbed differential equations (SPDEs). The prediction task is modeled as a regression problem and is solved using ANN. Three training strategies for the ANN have been proposed ie supervised, L2 error minimization (global) and L2 error minimization (local). It has been observed that the proposed method yields accurate results, and even outperforms some of the existing state-of-the-art ANN-based partial differential equation (PDE) solvers such as Physics Informed Neural Network (PINN).

Emerging topology and shape optimization techniques in computational design of materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NEURAL NETWORK-BASED TOPOLOGY OPTIMIZATION OF ACOUSTIC METAMATERIALS

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ABSTRACT

In recent years, substantial efforts have been dedicated towards designing acoustic metamaterials for noise attenuation across a broad frequency range. In that context, Multiresonant Layered Acoustic Metamaterial (MLAM) panels [1] offer noise attenuation at low frequencies (below 1000Hz) by leveraging the coupling effect between two resonant frequencies, resulting in notably increased noise attenuation compared to homogeneous material of equivalent mass.

This work proposes a two-phase strategy for the design of MLAM panels based on (1) a neural network-based surrogate model to efficiently assess the effective properties of individual layers computed from a homogenization approach, expediting the computation of the noise attenuation (measured as the Sound Transmission Loss), and (2) a topology optimization strategy to maximize the noise attenuation both in intensity and frequency range, while preserving a coupled STL response. The optimization strategy involves parameterizing the geometry of MLAM layers, and leveraging a genetic algorithm guided by the DNN-based models. The resultant optimized solutions exhibit noise attenuation exceeding 20 dB over 330 Hz in comparison to homogeneous materials with the same surface density.

The use of the proposed surrogate model results in enhanced accuracy in the prediction of effective properties and evaluation of the STL with respect to classical polynomial interpolation techniques, and a significant reduction in the computational cost of the optimizations when compared to direct numerical simulations, enabling cost-effective optimizations of multiple objective functions and constraints. [2,3]

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DARCY FLOW-BASED TOPOLOGY OPTIMIZATION FOR DESIGNING TWO-FLUID HEAT EXCHANGER OF A ROCKET ENGINE

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ABSTRACT

In this study, we present a three-dimensional topology optimization method aimed at enhancing the efficiency of a two-fluid heat exchanger of a rocket engine. Given the inherent complexity and nonlinearity of the original design problem, our methodology adopts a two-step approach inspired by the previous works [1–3]: first, a low-fidelity topology optimization utilizing a Darcy flow model for rapid and stable optimization, followed by a high-fidelity evaluation in the second step. The latter involves a forward analysis incorporating a turbulence model. The results reveal that the optimized design showcases distinctive characteristics, featuring intricate flow channels that set it apart from traditional heat exchangers.

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Verification techniques in computational physics and applied mathematics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NEW APPROACH TO CONSTRUCTING SOLVABLE PROBLEMS IN FREE VIBRATION EIGENVALUE PROBLEMS OF ELASTICITY

Takahiro Yamada[*1]*

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ABSTRACT

In various fields, dynamics problems of elastic bodies appear as structural vibrations or propagation of elastic waves. In this study, we propose a new approach to construct exact solutions of free vibration of elastic bodies and discuss the verification of numerical procedures using obtained exact solutions. Conventional exact solutions of eigenvalue problems are obtained by setting the domain and boundary conditions and searching for a solution that satisfies a partial differential equation. However, there are few problems for which the exact solution obtained by such an approach can be expressed explicitly.

In this work, two techniques are used to construct new problems with the exact solution expressed explicitly. One of them is to use the Helmholtz decomposition in elastic wave theory to decompose the problem into one expressed in terms of scalar eigenfunctions for P-wave and vector-valued eigenfunctions for S-wave. Another technique is to search for candidate eigenfunctions that satisfy the partial differential equation and derive the boundary conditions from the boundary values satisfied by these functions, instead of solving a problem with boundary conditions. From these candidate solutions, we select the ones with the numerically applicable boundary conditions and derive new problems for which exact solutions can be expressed explicitly. The obtained problems for rectangular and cylindrical domains are used to verify finite element schemes and to evaluate their numerical properties.

A CONTINUUM MATHEMATICAL MODEL FOR GENERATIVE DESIGN OF PLANAR MECHANISM

Yurika Sayo[1] and Takayuki Yamada[*1]*

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ABSTRACT

Topology optimization is a useful methodology for designing the shape of structures. However, when designing a mechanism such as a link mechanism, it is necessary to specify the positions of candidate links and joints in advance. In order to achieve a generative design of mechanisms with a higher degree of freedom, it is necessary to approximate the motion of the mechanism based on the framework of a continuous system, such as continuum mechanics. To achieve this objective, a new mathematical model will be formulated.

PSE (Problem Solving Environment)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT OF A SOCIAL SKILLS SCALE FOR CHINESE STUDENTS IN JAPAN AND JAPANESE STUDENTS IN CHINA

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ABSTRACT

The Japanese Ministry of Education, Culture, Sports, Science and Technology (MEXT) is currently focusing on the globalization of higher education. This involves emphasizing the acceptance and retention of international students, promoting Japanese students to study abroad, and fostering the development of global human resources. In light of these circumstances, research on the social skills of international students has garnered significant attention. Social skills encompass both verbal and non-verbal interpersonal behaviors employed to respond in social situations, as well as the cognitive processes that facilitate the expression of these interpersonal behaviors. Some studies suggest that cultural understanding is better promoted when international students and host country students engage in this social skills training together. The composition of international students in Japan is predominantly Chinese, while Japanese students often opt for study programs in Europe and the U.S. This pattern implies a limited interactive exchange between Japan and China. It has been pointed out that there are differences in social skills required depending on the country of origin, culture, and country of residence. The purpose of this study was to develop a social skills scale for Chinese students in Japan and Japanese students in China. This involved employing the Social Skills Self-Rating Scale for Adults employed in Japan and a condensed version of the Chinese University-Students Social Skill Inventory (ChUSSI), commonly used among university students in China. The survey was conducted by means of an online questionnaire. The survey involved a total of 139 participants from Japanese and Chinese universities. Among them, 82 were Chinese students, and 57 were Japanese students. As a result of factor analysis using the principal factor method and promax rotation, six factors were extracted and named "inferring others," "expressing opinions," "initiating conversation," "relationship maintenance," "partner’s face," and "emotional control,". Cronbach's alpha coefficients were α=.85, .76, .78, .75, .72, and .75, respectively, indicating high internal consistency. The above results suggest the reliability of the created scale. There were factors that were compatible with the factor items of the Japanese version of social skills, suggesting construct validity. In the future, we envision the application of the social skills identified in this study to the development of social skills programs and international student education initiatives. This will involve a thorough examination of the specific contexts in which these social skills are most needed.

Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HYPERELASTIC CONSTITUTIVE MODELS FOR GEOMATERIALS IN SMALL STRAIN AND FINITE STRAIN: A REVIEW FROM THE ASPECT OF STABILITY

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ABSTRACT

This study is concerned with the stability/instability property of hyperelastic models for geomaterials. We first present the reformulation of several existing representative hyperelastic models for geomaterials with pressure-dependent bulk and shear moduli within the frameworks of small strain and finite strain. In finite strain formulation, the stress versus elastic strain relation, together with the fourth-order elastic tangent moduli tensor, in the description relative to the intermediate configuration is derived for each of the hyperelastic models. Their spatial and material descriptions are also derived. These descriptions are compatible with the multiplicative finite strain elastoplasticity. A systematic parametric study with a particular focus on the pressure-dependent property of the elastic moduli was performed to examine the constitutive response of the hyperelastic models and compare the small strain models and the finite strain models under typical cases of simple shear, pure shear, and triaxial (axisymmetric) compression. The analysis revealed significant differences in the model responses depending on the types of model, as well as on the value of material constants related to the pressure-dependency of elastic moduli. Notably, some models exhibited unexpected unreasonable decreases in stress during triaxial (axisymmetric) compression. We then examined the property of the hyperelastic models from the viewpoint of stability/instability to elucidate the mechanical cause of the above-mentioned decrease in stress. The stability criterion is defined by the positive-definiteness of the fourth-order elastic tangent moduli tensor. We therefore performed eigenvalue analysis of the elastic tangent moduli tensor, and thereby confirmed consistent correspondence between the increase/decrease in stress and the stability/instability of the material. We also discuss the significance of elasticity in the numerical computation of elastoplasticity when a hyperelastic model is combined with plasticity. Numerical examples are presented to demonstrate the important role of elasticity in providing an elastic predictor within the return-mapping scheme.

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Predictive digital twins
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STRUCTURAL MODEL UPDATING OF STEEL FRAME FOR DISPLACEMENT PREDICTION DURING CONSTRUCTION USING DATA-DRIVEN APPROACH

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ABSTRACT

In the construction of steel frame structures such as dome structures, numerical simulation of the structural steel erection work is conducted, and its appropriate order is determined to ensure structural stability during the construction process. However, discrepancies arise between the simulation results and observation results due to the errors related to construction accuracy. We are working on the development of a digital twin for building construction to accurately predict the behavior of structure in the process of steel erection work. Our framework employs a data-driven modeling approach to obtain the as-built model of the structure, which includes uncertainties concerning construction accuracy.
The feasibility of the proposed framework was tested using the measurement data set acquired during the construction of an actual dome structure. Based on the results of preliminary welding experiments and sensitivity analyses of the parameters in the structural model, the error sources of the as-built model were considered to be mainly derived from weld shrinkage at the joint of steel beams and the stiffness of the temporary roof support system. These properties were treated as identifying parameters with uncertainties. We sequentially updated the probability distribution of the parameters by assimilating displacement data provided from position measurements with ensemble transform Kalman filter. The displacement caused by the subsequent steel erection works was predicted by the updated model with uncertainties. The result shows that the proposed framework can reduce the prediction error compared to the conventional model without data-driven modeling.

Buckling analysis and design of thin-walled structures based on novel and intelligent computational methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BUCKLING OF SHELL STRUCTURES BY USING THE NOVEL APPROACH

Takeki Yamamoto[1] and Takahiro Yamada*[2]

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ABSTRACT

Shell structures are used in a wide range of fields for pressure vessels, storage tanks, submarines, and aircraft fuselages. In these structures, buckling may occur due to various loading, such as compression, bending, twisting, shearing, and internal and external pressures. For the purpose of evaluating the buckling behavior accurately, it is important to pursue the equilibrium paths. When the internal and external pressures are applied to both the top and bottom surfaces of shell structures, the behavior is different from the case where the pressure acts on either one surface.
Buckling phenomena of structures under pressure load are investigated using the finite element analysis. Toscano et al. proposed the finite element model discretized with shell elements for analyzing the buckling and buckling propagation of stiffened pipes, and verified the model by comparing the numerical results with the experimental one [1]. In this approach, the pressure load is evaluated at the midsurface of the structure. On the other hand, Zhu et al. presented the numerical calculation considering the three-dimensional finite deformation for the thick-walled cylindrical shell to evaluate the pressure load appropriately in the buckling analysis [2]. However, it needs huge computational costs in evaluating the complicated behaviors using continuum elements.
In this work, we propose a novel approach to evaluate the buckling behavior in the framework of structural elements. This approach is based on the conventional shell element, and applied to the special shell element, in which the external force is directly given to the additional nodes representing the thickness-stretch [3]. In this approach, the number of unknowns in the resulting linear system of equations coincides with that of the conventional shell elements. In the situation that a perturbative load is applied under a certain stress state, bifurcation points are searched by solving a standard eigenvalue problem.

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Current trends in phase-field modeling and computations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IDENTIFICATION OF PARAMETERS INCLUDED IN PHASE-FIELD FRACTURE MODEL USING BAYESIAN DATA ASSIMILATION AND DIGITAL IMAGE CORRELATION

Akinori Yamanaka[*1], Ryuki Funamoto[1], Kengo Sasaki[1] and Akimitsu Ishii[2]*

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ABSTRACT

Prediction of crack propagation and failure of the material are essential for designing engineering components. However, experimental direct observation of crack propagation inside a material is difficult. Therefore, numerical simulation of crack propagation behavior using a phase-field fracture (PFF) method has attracted much attention. On the other hand, the PFF models often require multiple parameters (e.g., interface mobility and interface energy) which are challenging to be identifed from experimental data. In this study, we develop a new data-driven method to estimate the parameters included in the PFF model by integrating experimental data and the model based on data assimilation based on Bayes' theorem (i.e., Bayesian data assimilation) [1]. In this study, the developed method was used to simulate the time evolution of crack propagation behavior and strain evolution of an asymmetrically notched aluminum alloy sheet specimen. The full-field strain evolution on the surface of the specimen obtained by the digital image correlation method was assimilated to the PFF model [2] using the DMC-TPE method [3, 4]. The results demonstrate that the parameters related to the fracture toughness and three parameters of the strain hardening law were successfully estimated.

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Phase-field modeling: Analytics, benchmarks, and discussions
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

3D MULTI-PHASE-FIELD LATTICE BOLTZMANN SIMULATIONS FOR SEMI-SOLID DEFORMATION IN THIN FILM

Namito Yamanaka[*1], Shinji Sakane[1] and Tomohiro Takaki[1]*

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ABSTRACT

In the casting process, semi-solid deformation induces the formation of solidification defects such as band segregation. Thus, it is essential to thoroughly evaluate the semi-solid deformation behavior. Currently, X-ray in-situ observations have enabled the evaluation of the interaction between moving grains during semi-solid deformation, and it has been reported that the deformation behavior is dominated by grain rearrangement. However, the fluid flow that strongly affects grain rearrangement cannot be observed. Thus, numerical simulation is indispensable, whereas the simulation studies are insufficient, and no definitive method has been developed yet.
In our previous study [Comp. Mater. Sci. 197 (2021) 110658], a multi-phase-field lattice Boltzmann (MPF-LB) model was developed to evaluate polycrystalline solidification with fluid flow and grain motion, and was applied to semi-solid deformation. In the MPF-LB model, the contact between grains was modeled by considering the overlap between the phase-field variables, and the solid walls were modeled using phase-field variables as a solid. Through this model, semi-solid deformation with various deformation conditions was simulated. However, all simulations were limited to two dimensions. In this study, the MPF-LB model is extended to three-dimensional problems, and simple shear deformation in thin film is evaluated. Through systematic 3D MPF-LB simulations of semi-solid simple shear deformation, the relationship between solid grain rearrangement and fluid flow is investigated in detail.

Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SURROGATE COMPUTATIONAL HOMOGENIZATION FOR COMPOSITES CONSISTING OF MULTIPLE VISCOELASTIC MATERIALS WITH TIME-TEMPERATURE SUPERPOSITION PROPERTIES

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ABSTRACT

We propose a surrogate computational homogenization for viscoelastic composites by means of RBF interpolation. Nowadays, mechanistic machine learning techniques (MMLT) is incorporated into the field of computational mechanics to realize or accelerate numerical simulations for complex phenomena. The multiscale problem is one of the targets of the application of MMLT, by which several studies have achieved micro-macro two-scale analysis of composite nonlinear materials with less computational cost than that of conventional methods; see, e.g., reference [1]. To the best of our knowledge, those studies mostly owe a class of neural network, one of the deep learning methods. However, from a mathematical point of view, deep learning does not have significant advantages over shallow learning such as kernel methods in representing continuous function [2]. Therefore, NNs are not necessarily the best method for predicting mechanical behavior because the nonlinear multiscale problem is completely continuous. In this regard, we employed radial basis function (RBF) interpolation, a shallow learning method to globally interpolate a lot of discrete data as was done in our previous study[3], to create a surrogate model that can replace the entire microscopic analysis in the two-scale problem of viscoelastic composites. In other words, the macroscopic stress of a viscoelastic composite is represented by the created surrogate model in consideration of the dependencies on strain rate and temperature.

The proposed method is validated through numerical examples. First, by conducting numerical material tests (NMTs) on a representative volume element consisting of multiple viscoelastic materials, we obtain a data set representing the macroscopic constitutive relationships for various deformation patterns. Second, using the data set, we create a surrogate model by performing RBF interpolation. Third, for validation purposes, the responses of the surrogate model are compared with the results of NMT that has been performed with unseen loading and temperature histories. Finally, a FE analysis is performed as macroscopic simulation by utilizing the surrogate model, and the result is compared with that obtained by direct numerical simulations to demonstrate the validity of the present methodology.

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Emerging topology and shape optimization techniques in computational design of materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NOVEL METHOD FOR DESIGNING STIFFENERS BY SIMULTANEOUS OPTIMIZATION METHOD OF SHAPE AND TOPOLOGY

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ABSTRACT

Stiffeners are structural elements with superior mass-to-stiffness ratio and are widely utilized in the engineering structures. Determining the optimal layout and size of stiffeners without relying solely on the designer's intuition has attracted much attention in recent years. Previous researches have focused on finding the optimal layout under the pre-prepared height and thickness or optimizing the height and thickness under the pre-prepared layout.

In this study, we propose an optimal stiffener design method that automatically finds the optimal layout and shape of stiffeners at the appropriate locations without any prior preparation from a bulk solid structure using simultaneous optimization method of shape and topology. A SIMP (Solid Isotropic Material with Penalization) based topology optimization method is used for strategically placing stiffeners within the specified design domain, while the non-parametric shape optimization method is used for determining the optimal shape of stiffeners. The objective function, compliance, is minimized under several constraints; the equilibrium equation for designing the stiffener, the total volume, the maximum height and the width. A fictitious equilibrium equation is also introduced to control the width of the stiffeners efficiently.

After formulating this simultaneous design optimization problem, the shape and density sensitivity functions are derived using the Lagrange multiplier method and the adjoint method. The shape and density sensitivity functions are applied to the vector-type(1) and the scalar-type H1 gradient method(2),(3), respectively, which provides the detail determination of optimal shape and topology. The introduction of the both types of H1 gradient method serves a dual purpose, enabling the achievement of a smooth optimal external shape of the stiffeners while concurrently addressing inherent issues related to grayscale and checkerboard patterns, as well as reducing the objective function. Several numerical examples prove the effectiveness of the proposed method.

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PSE (Problem Solving Environment)
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE INFLUENCE OF FAMILY ENVIRONMENT ON PERSONALITY

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ABSTRACT

Introduction
Research on human character and personality has been ongoing for many years. A frequently debated question is how these personalities are formed. It is now common to believe that heredity and environment mutually influence personality through experiments with twins. The family environment is often cited as an environment that influences personality. One well-known example is Bowlby's attachment theory. This theory suggests that attachment relationships in infancy also influence future relationship formation and psychological health. The purpose of this study is to investigate the family environment on personality and to consider the causes of the influence to help discover and develop methods to reduce the unfavorable influence of the family environment on personality.

Method
Approximately 130 male and female undergraduate and graduate students, both physically and mentally healthy, attending Toyo University participated in the study. A psychological test using the Tokyo University Egogram TEG and a questionnaire survey using a domestic atmosphere diagnostic test will be conducted together to examine the correlation between the two.

Result
Overall correlation and multiple regression analyses did not show these relationships. However, in the Nurturing Parent (NP) dominant group, Free Child (FC) and warmth in the home and Adapted Child (AC) and brightness in the home were moderately correlated. Approximately 30 other combinations showed moderate correlations (0.4 or higher).

Conclusion Discussion
Persons with low FC are generally considered to be depressive. Although limited to the NP-dominant group, a warm and democratic home environment can be expected to foster a high FC personality. It was suggested that FC could be enhanced by increasing warmth and democracy in the home. Also, by examining the impact of these influences, it may be possible to find factors that increase or decrease FC.

Further challenges
The number of samples was too small to examine the correlations in many cases, but discoveries may be made in the future when a larger number of samples are secured and correlations are examined. It is also necessary to investigate the causes of the influence of the family environment on personality in the future.

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SURROGATE MODELING FOR EFFICIENT SEISMIC DISASTER SIMULATION USING DETAILED FINITE ELEMENT ANALYSIS

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ABSTRACT

We have developed an E-Simulator, a numerical simulation designed to replicate the damage and collapse behavior of structures during major earthquakes. Given the high computational cost, using the E-Simulator for regional seismic disaster prediction is impractical. To address this, we are developing a surrogate model for detailed finite element (FE) analysis of building structures.

Surrogate modeling using machine learning is a growing field, but generating large training datasets for large-scale simulations is challenging. Our approach trains individual components of the target structure, allowing us to generate a feasible dataset and assemble these components into a complete structural model.

This study introduces a surrogate model for a structural member unit consisting of beams, columns, and a connection. We employ a recurrent neural network with proper orthogonal decomposition to reduce the dimensionality of the neural network's input and output nodes. The model effectively replicates physical fields such as displacement, stress, and strain from nonlinear FE simulations, maintaining high accuracy with minimal loss.

Our work demonstrates the potential of surrogate models in computational mechanics, offering a practical solution for large-scale structural simulations in seismic response analysis.

Advances in neural operators for scientific modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A PHYSICS-INFORMED OPERATOR LEARNING FRAMEWORK INSPIRED BY THE FINITE ELEMENT METHOD FOR PREDICTION OF DYNAMICS PHYSICAL PHENOMENA: CASE STUDY ON TRANSIENT HEAT CONDUCTION

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ABSTRACT

In this study, we present a novel physics-informed operator learning framework that allows for predictions of evolutionary physical phenomena described by a time-dependent partial differential equation using a loss function inspired by the finite element method (FEM). Transient thermal conduction is considered to demonstrate the performance of the present framework. For the thermal problem, the networks take a temperature field at the current timestep as input and predict a temperature field at the next timestep. The Galerkin-discretized weak formulation of the heat equation is employed to incorporate physics into the loss function, which is coined finite operator learning (FOL) [1]. Furthermore, we introduce an additional term to the loss function with the aim of restricting the evolution speed of temperature fields over time. After sufficient training, the networks successfully predict temperature evolution over time for unseen cases even after multiple timesteps at high accuracy compared to the solution by FEM. We also confirm the applicability of the framework to cases with heterogeneous heat conductivity and various timestep sizes.
The advantages of the proposed FOL framework are summarized in the following two points: first, the training of the networks is performed completely in an unsupervised manner, in which, in contrast to data-driven deep learning models, one does not need to prepare a huge data set from costly simulations or experiments. Instead, a data set of random temperature patterns generated by the Gaussian random process and the Fourier series in combination with constant temperature fields is used as training data to cover a wide range of possible temperature cases. The other important feature is that shape functions and backward difference approximation are exploited for spatial and temporal discretization, respectively, resulting in a pure algebraic equation analogous to data-driven loss functions. This allows for enhancing training efficiency, as one avoids time-consuming automatic differentiation when optimizing weights and biases.

The present FOL framework for dynamic systems could be extended to other types of dynamic partial differential equations, such as the Allen-Cahn and Cahn-Hilliard equations that describe dynamic phase separation.

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Predictive digital twins
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN DIGITAL TWIN FOR DYNAMIC STRUCTURES BASED ON REDUCED-ORDER MODELS AND MACHINE LEARNING

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ABSTRACT

A data-driven method for digital twin of dynamic structures based on reduced-order models and machine learning algorithm is proposed. High-fidelity finite element (FE) models reflecting the undamaged and damaged states of a physical structure during service are established, and model order reduction method is then used to project all the high-fidelity FE models into reduced-order models. A dataset is created from the numerically simulated dynamic responses of the reduced-order models under calibration loads. Using the numerically determined strains at the locations where sensors will be placed on the physical structure as input data, a machine learning algorithm is used to train the model selector, which will infer the real-time state of the physical structure during service utilizing the sensor data. Digital twin based on the Krylov subspace model order reduction method and the random forest algorithm is presented. Physical structure of a spatial frame was built to experimentally and numerically illustrate the efficiency of the digital twin. Effects of the difference among various states of the structure, sensor arrangement and calibration load on the classification accuracy of the trained model selector are investigated. It is discovered that: (1) The presented method is suitable for structures subjected to dynamic load, and the Krylov subspace model order reduction method is efficient for reducing the order of structural dynamic equations. (2) The digital twin can be updated online if its response time is shorter than the sensor sampling time, and can be updated offline if its response time is longer than the sampling time. The digital twin can operate during any period of time and in any damaged and undamaged state during structure service. It is not necessary to operate the digital twin uninterruptedly. (3) The amplitudes and frequencies of calibration loads should cover all the possible values of the excitation loads the structure subjected to during service. (4) Sensor arrangement scheme play a key role for the classification accuracy of model selector. The closer the sensors to the damage zone the better the accuracy. Sensors far away from the damage zone are not beneficial and even jeopardize the accuracy. (5) The effects of uncertainties regarding material properties and geometrical features of the structure, operation parameters, loading and environment as well as noise in sensor data need to be studied in the future.

Immersed-boundary variational methods: Theory, data structures, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LEVEL-SET ASSISTED ENRICHED IMMERSED BOUNDARY METHOD FOR STEFAN PROBLEM WITH APPLICATIONS TO ADDITIVE MANUFACTURING

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ABSTRACT

Stefan problem is ubiquitous in many engineering problems such as welding, heat exchangers, and additive manufacturing. However, it is challenging to solve Stefan problem involving the moving material interface with conventional numerical methods while preserving boundary accuracy and mesh flexibility. In this talk, we introduce the level-set assisted enriched immersed boundary method to track the fluid-solid interface and enforce the critical Neumann boundary conditions accurately on the material interface. The main feature is to generate the interfacial surface which is independent of the volumetric computational domain with a level-set field based on the Neumann boundary condition for the fluid-solid interface and duplicates the DoFs at the interfacial domain to enforce Dirichlet and Neumann boundary conditions. We will present a set of examples to show the proposed approach in phase transition problems and additive manufacturing and the comparison it with existing methods will be also presented.

A REPARAMERIZATION OF TOPOLOGY OPTIMIZATION USING PINN AND CNN FOR STRESS AND FREQUENCY OPTIMIZATION

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ABSTRACT

Topology optimization (TO) represents a forefront methodology in structural optimization, facilitating the discovery of innovative and optimally tailored structural solutions. These solutions cater to diverse objectives and constraints, while not being bound by preconceived shapes. However, TO's application is predominantly confined to high-integrity or small-scale structures, constrained by its substantial computational demands and limited capabilities in managing complex objective/constraint functions. Additionally, as a non-convex optimization problem, TO's solution optimality can be further enhanced through achieving superior local optima.

This work address these TO challenges by integrating machine learning (ML) techniques, specifically focusing on accommodating complex objective functions such as p-norm von Mises stress and eigenvalues. The integration of various ML approaches into TO has been explored, ranging from models that predict structural responses to comprehensive ML strategies that directly optimize designs. Informed by the pioneering work of Hoyer et al. [1] and Zhang et al. [2], this study introduces a novel reparameterization of topology optimization utilizing physics-informed neural networks (PINNs) and convolutional neural networks (CNNs). This approach is devised to simultaneously minimize the maximum von Mises stress and maximize the first natural frequency of structures.

Significant reductions in computational cost have been achieved through the implementation of advanced sparse solvers and modified constraint handling techniques. The newly implemented reparameterization has led to the discovery of enhanced designs for both stress-based and vibration-based TO applications, showcasing the potential of ML in pushing the boundaries of traditional topology optimization.

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Current trends in phase-field modeling and computations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SIMULATION OF ROLLING CONTACT FATIGUE UTILIZING A PHASE FIELD MODEL

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ABSTRACT

Fatigue failure is one of the most crucial issues in manufacturing and engineering processes. Repeated cycles can cause cracks to form and grow over time, eventually leading to structural failure. To avoid these failures, it is important to predict fatigue crack growth by simulation methods. In the past decade, the phase field method for fatigue fracture has drawn a lot of attention for its uniform description of complicated crack evolution behaviors. However, there is still a lack of studies on the applicability to industrial problems. In this work, we use the phase field fatigue model to analyze the rolling contact fatigue tests.

Data-driven approaches for solid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A DISTRIBUTED COMPUTING FRAMEWORK FOR MODEL-FREE DATA-DRIVEN METHODS

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ABSTRACT

Model-free data-driven methods provide a new computing diagram for solving boundary value problems (BVP) in computational mechanics[1]. This paradigm can bypass the explicit material modeling by directly incorporating material data into BVP solution. The computational complexity of this paradigm mainly arises from data search, especially in high-dimensional phase space. However, the amount of material data required for the data-driven computing grows exponentially with the number of dimensions. The dramatic increase in data volume and computational complexity exceeds storage and computing capabilities of most single PC. To overcome such a problem, we have developed a distributed computing framework for model-free data-driven methods.

The distributed computing framework can coordinate multiple computers to process high-dimensional data. The Hadoop Distributed File System (HDFS)[2] is introduced to split a large-scale material dataset into small data blocks and store them on different computers. The MapReduce computing engine[3] is used to process material data search in parallel on multiple computers. First, a global data search task is mapped to each data block with excuting the local distance calculations in parallel. Then, all local distance data are aggregated and sort. Finally, the results are merged into the output of the global nearest data and the minimized distance.

A 3D elasticity test case was used to examine the performance of the distributed computing framework built on a cluster of three computers. As the size of datasets increases, the advantages become apparent due to parallel computation on multiple computers. We used this distributed framework to perform the data-driven computing on a material datasets up to 400 million points of twelve-dimensional data. This work shows that the distributed computing framework is essential for developing the model-free data-driven algorithms for large-scale high-dimensional problems.

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Computational mechanics for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HIGH-FIDELITY MODELING OF MULTI-MATERIAL ADDITIVE MANUFACTURING

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ABSTRACT

Additive manufacturing possesses promising capabilities of fabricating new materials by mixing multi-material powders and manipulating chemical compositions. In this talk, we will present our latest work on high-fidelity modeling of the complex additive manufacturing process: from powder spreading to melting. To evaluate the mixture uniformity of the powder layer/stream, we employ the computational fluid dynamics (CFD) and discrete element method (DEM) coupling method to simulate the powder spreading/blowing processes of mixed multi-material powders. To thoroughly understand the material composition distribution in the melting procedure, we develop a multi-physics thermal-fluid flow model to simulate the different melting/flow/solidification behaviors of different powders as well as the interactions between solid powders and molten pool. Various scenarios are simulated from micro-/nano-particle reinforced composites to in-situ alloying for new materials. All these models are validated against experiments, and show appealing potentials to provide guidance for additive manufacturing of mixed powders.

Machine learning and data driven based engineering computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTI-PHYSICS FIELD-DRIVEN INVERSE DESIGN AND MANUFACTURING FRAMEWORK FOR MECHANICAL METAMATERIALS ACCELERATED BY NEURAL OPERATORS

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ABSTRACT

Mechanical metamaterials derived from phase separation patterns of spinodal decomposition have garnered attention due to their lightweight, high-strength and tunable mechanical properties. Generally, the spatiotemporal evolution of spinodal decomposition can be characterized using the Cahn-Hilliard equation. However, the computational challenges in numerically solving the 3D Cahn-Hilliard equation, such as high computational complexity and the need to maintain numerical stability, significantly impede the design of the metamaterials with desired mechanical properties. To overcome these challenges, this study proposes a multi-physics field-driven inverse design and manufacturing framework significantly enhanced by advanced neural operators. A Cahn-Hilliard with anisotropic diffusion parameters is utilized to analyze the solution patterns in the frequency domain through Fourier transformation. Then, a novel Fourier neural operator model is developed to simulate diverse anisotropic phase separation patterns, accounting for varying diffusion parameters, initial conditions, and boundary conditions. Specifically, the architecture of the model uniquely combines three-dimensional spatial field transformation in the frequency domain with temporal encoding using the self-attention mechanism, ensuring rapid and accurate prediction of concentration fields. This approach directly integrates anisotropic diffusion parameters, initial conditions, and boundary conditions as model inputs, enabling it to predict concentration fields across various time points with remarkable computational efficiency and accuracy, representing a significant leap over traditional numerical methods of PDEs. Moreover, the relationship between phase separation patterns and desired mechanical properties is discussed. Utilizing anisotropic diffusion parameters and evolutionary time as inputs, a multilayer perceptron (MLP) based on physical parameters is built to predict the corresponding mechanical properties, facilitating inverse identification of optimal diffusion and evolutionary time parameters through a proposed global optimization algorithm. The practical application of the proposed method in metal additive manufacturing is demonstrated, particularly in fabricating personalized medical implants from Ti6Al4V tailored to match the orthotropic mechanical properties of natural bones. The proposed method achieves a rapid, physics-driven inverse design, eliminating inexplicable design variables of traditional generative machine methods and substantially improving generalization performance. This study establishes a new paradigm in designing and manufacturing mechanical metamaterials derived from parametric PDEs, offering a robust and efficient pathway for broad application across engineering fields.

Extended digital twins including uncertainty and complexity of human/society and human knowledge
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTATIONAL EMOTION MECHANICS AND INQUIRY PROCESS

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ABSTRACT

Inquiry stands as an essential human activity embedded in scientific research, creation and education, steered by emotions such as curiosity and interest. We propose a mathematical model encapsulating these emotions, using information gains derived from the principle of free energy minimization. Free energy, representing prediction errors with the uncertainty inherent in the Bayesian brain, diminishes through recognition and learning, generating information gain and inducing positive emotions. The psychological concept of arousal potential indicates that an optimal level of arousal induces positive emotions. Two kinds of curiosities are identified, namely diversive and specific, which are instrumental in achieving the optimal arousal level that maximizes positive emotion. Free energy or surprise signifies emotional arousal. We model the curiosities using information gains resulting from reductions in free energy during recognition and learning. We propose that the alternate maximization of these information gains defines an ideal inquiry cycle, guiding toward the optimal arousal level, with curiosity serving as the driving force propelling this cyclic process. By employing the Gaussian generative model supplemented by a uniform likelihood, we found that information gains manifest as an upward-convex function of arousal (surprise) with an optimal arousal level. We comprehensively analyzed the effects of prediction uncertainty (prior variance) and observation uncertainty (likelihood variance) on the peaks of the information gain function, considered as optimal surprises. The results show that greater prediction uncertainty, indicative of an open-minded attitude, and reduced observational uncertainty, signifying precise observation with focused attention, are expected to provide greater information gains across a broader spectrum of exploration. The proposed mathematical framework unifies the free energy principle of the brain and the arousal potential theory. It explicates emotional valence as an information gain function, proposing an idealized inquiry process driven by epistemic emotions.

Computational modeling of extreme-loading events
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL MODEL OF A STEEL END-PLATE MOMENT CONNECTION USING A NOVEL CYCLIC LOADING PROTOCOL

Jorge Pi Luco[1], Sergio Yanez[1], Miguel Medalla Riquelme[2], Juan Carlos Pina[1] and Carlos Felipe Guzmán[1]*

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ABSTRACT

Bolted connections are an efficient solution for erecting steel elements in buildings and industrial structures in regions with high seismic activity. The performance of these connections depends on factors such as the number of bolts, the thickness of the plate, the presence of stiffeners, and others, which can cause the connection to fail in a brittle or ductile manner. This performance is even more crucial when earthquakes occur in subduction zones. Given their profound impact on structural performance, there is a pressing need for research into novel moment connection configurations. This study addresses this gap by proposing a new loading protocol tailored to assess the performance of bolted end plate moment connections under the damage induced by mega-earthquakes in subduction zones. Through numerical modeling, bolted moment connections subjected to both monotonic and cyclic loads are analyzed using the finite element method. The loading protocol introduces an alternating vertical displacement at the free end of the beam, progressively increasing in amplitude between load steps. Contact interactions between connected parts allow for separation between the end plate and the column flange. An increase in the Plastic Deformation Index (PEEQ) was observed when the plate thickness is reduced by 25%. Furthermore, the Rupture Index (RI) exceeds unity for all bolts, indicating crack formation. A novel loading protocol that integrates the damage caused by mega-earthquakes in subduction zones offers a comprehensive understanding of the structural response of various steel beam-column bolted end-plate connections with diverse bolt configurations. Finally, the stress-strain response of the connections was obtained to propose new design considerations for seismic-resistant structures.

Computational mechanics in high-strain rate and impact engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FAILURE DAMAGE ANALYSIS OF UHWMPE/PET FOAM SANDWICH STRUCTURES UNDER HIGH-VELOCITY IMPACT

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ABSTRACT

The present work deals with the high-velocity impact (HVI) behaviour of composite sandwich structures based on experimental and numerical method. The composite sandwich structure consists of two ultra-high molecular weight polyethylene (UHWMPE) laminates and a PET (polyethylene terephthalate) foam core. A series of HVI tests were conducted on the UHWMPE/PET foam sandwich structures to investigate the HVI performance and damage mechanisms. Micro-computerized tomography (μCT) characterization method was used to detect the internal damage patterns in the sandwich structures. A finite element model (FEM) was developed which Puck's failure criteria simulates intra-layer failure, cohesive law simulates inter-layer failure and the crushable foam plasticity model combined with ductile damage criterion simulates the foam failure. After validation of the proposed model by experimental results, the damage mechanism of the sandwich structures under HVI loading was examined, and the effects of impact velocity on the failure patterns and residual velocity were discussed.

Several key conclusions from this study are summarised as follows:
1. Circular hole-type damages were only observed on the upper panel, even though the impactor penetrated the composite sandwich structure. On the lower panel, only linear crack-type damage along the fibre direction were generated due to the rebound of the stretched fibres after the impactor penetrated.
2. Generally, the peak impact force and energy absorption values increase with higher impact velocity. However, when the impact velocity is less than the critical value (Critical velocity =200 m/s for the composite sandwich structure in the study), both the impact force load and energy absorption values remain relatively stable and are not significantly influenced by variations in impact velocity.
3.Foam cores in composite sandwich structures generate an upward rebound force during HVI when they are compressed to a certain extent, resulting in the appearance of a third peak in the impact load curve and absorbing more energy.
4.The presence of UHMWPE fibre interspersed in the panel tended to inhibit the spread of damage in the impacted region. Only matrix tension damage showed noticeable propagation during HVI, and matrix tension damage increased with the impact velocity, reaching a plateau when the velocity exceeded 250 m/s.

DTN BOUNDARY CONDITION BEM AND FEM

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ABSTRACT

Wave scattering emerges in many applications such as sonar, radar, antennas, seismic exploration, crack detection, satellite imaging, and microscopy. Dirichlet-to-Neumann boundary conditions (DtN bc) are often encountered in wave scattering calculations. By effectively handling DtN nonreflecting bc, the amount of computation is reduced to a certain extent, and the stability and accuracy of calculation will be significantly improved. These advantages are further amplified especially in high-frequency computations. In this paper, DtN boundary condition BEM and FEM are proposed in typical infinte structures, such as infinitely long pipe, infinite plate, half-space and infinite domain. In our proposed method, DtN boundary condition at artificial interfaces will be used to construct the linear mapping matrix of displacement and force, which will be incorporated into BEM and FEM as a modified term.

Advance and application of meshfree methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A STABILIZED MIXED-FORM MATERIAL POINT METHOD FOR FREE SURFACE FLOW MODELING

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ABSTRACT

The material point method (MPM) can effectively model engineering problems under large structural deformation with potential material separation. The Lagrangian particle description, adopted with a background Eulerian-style approximation in MPM, bypasses the mesh entangling issue commonly seen in mesh-based approaches. However, when MPM is applied to free surface flow problems with Navier-Stokes equations, it may suffer from volumetric locking and pressure oscillation due to the imposition of the incompressible condition, similar to other conventional numerical methods. In addition, the well-known MPM cell-crossing effect will affect the solution accuracy. To address these issues, a stabilized Galerkin mixed-form MPM is proposed to circumvent the numerical artifacts arising from incompressibility. Furthermore, the locking issue can be relaxed by revisiting the semi-Lagrangian kinematics [1] of MPM, deriving a corrected velocity update scheme. Last but not least, the reproducing kernel (RK) approximation [2] is employed to mitigate cell-crossing instability. The proposed algorithms are proven to be effective in solving a series of benchmark problems.

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Immersed-boundary variational methods: Theory, data structures, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SHIFTED BOUNDARY METHOD FOR FLOW SIMULATIONS OVER COMPLEX OBJECTS

Cheng-Hau Yang[1], Guglielmo Scovazzi[2], Adarsh Krishnamurthy[1] and Baskar Ganapathysubramanian[1]*

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ABSTRACT

The Shifted Boundary Method (SBM) [1, 2] is a novel variant of the immersed method to perform simulations in complex domains without using boundary-fitted meshes. Traditional computational fluid dynamics (CFD) methods face challenges in mesh generation and imposing boundary conditions accurately due to complex geometries. SBM addresses these issues by applying boundary conditions on a surrogate boundary with the boundary conditions changed appropriately using Taylor expansions. Conventional immersed boundary methods, such as the Finite Cell Method (FCM) and Immersogeometric Analysis (IMGA), require integration at the true boundary. On the other hand, in SBM, the boundary conditions are imposed by integrating at the Gauss points along a surrogate boundary, which aligns with the existing mesh structure. Additionally, SBM avoids the requirement of adaptive quadrature in intercepted elements, a common requirement in FCM and IMGA for accurate volume integration, thus simplifying the parallel implementation process. One of the standout benefits of SBM is its capability to resolve the issue of sliver cut cells, which often leads to poor conditioning of the stiffness matrix and challenges in numerical stability in other methods.

Recent advancements in SBM have extended its application to octree mesh frameworks [3], revealing the crucial role of selecting an optimal surrogate boundary in minimizing the error. This optimization has demonstrated significant benefits in solving Poisson and linear elasticity equations. In this study, we extend the application of SBM to tackle the Navier-Stokes equation using octree-meshes and an optimal surrogate boundary. We validate the method's efficacy through fluid dynamics benchmark cases, including flow around circular geometries and spheres, lid-driven cavity flow with a circular obstacle, and various aerodynamic problems at different Reynolds numbers. Our findings underscore SBM's robust capacity to address complex geometries in solving Navier-Stokes equations, showcasing its potential as a powerful tool in the realm of CFD for tackling complex geometries.

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Uncertainty quantification and reliability analysis in engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PROBABILITY DENSITY INTEGRAL EQUATION FOR UNCERTAINTY PROPAGATION AND TIME-VARIANT MOMENT FUNCTIONS OF STRUCTURAL RESPONSES

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ABSTRACT

Stochastic dynamic system follows the principle of probability conservation, which means when the randomness of system propagates and evolves from the input to output response, the probability measure determined by initial random source remains invariant. The principle of probability conservation presents two kinds of form, namely stochastic differential form and integral form. Based on the principle, this paper derives the probability density integral equation (PDIE) which is a stochastic integral form by using two ways. Then, several typical probability density evolution equations are derived through PDIE, namely, the Liouville equation, Fokker-Planck-Kolmogorov equation, Dostupov-Pugachev equation, and generalized probability density evolution equation, which are stochastic differential equations. This derivation reflects that the PDIE is fundamental equation characterizing the randomness propagation of system. Further, new time-variant moment functions of the system response are deduced from PDIE. Moreover, the calculation formulas of correlation functions of several random responses with multiple instants in input space are given for the first time. Finally, typical examples verify the correctness of the derived formulas and demonstrate the time-varying moment functions of responses of interest.

Multiphysics and data-driven modeling for cardiovascular biomedicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN METHODS FOR THE DIAGNOSIS OF CORONARY MICROVASCULAR DISEASE FROM ANGIOGRAPHY DATA

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ABSTRACT

Coronary microvascular dysfunction (CMD) is caused by impaired microvascular vasodilatation, leading to insufficient supplement of blood, oxygen, and nutrients to the myocardium [1]. The index of microcirculatory resistance (IMR) serves as a quantitative measurement of coronary microcirculatory function, and is currently considered as the gold standard [2]. Despite its benefits, the invasive nature of IMR assessment using an intravascular guide wire has led to its underutilization in current clinical practice. Consequently, a non-invasive, computationally efficient approach for accurate IMR assessment is highly desired.

In this study, a data-driven framework is proposed to (1) leverage the information encapsulated within angiography data, the primary modality for assessing coronary artery disease, and (2) computationally assess IMR based on angiography data. A multi-physics computational fluid dynamics (CFD) model of contrast injection is developed and calibrated to generate computational angiography data, providing a tool to interpret the dynamics of the contrast injection and washout within the coronary arteries. An encoder-based convolutional neural network is constructed to learn the correlation between the dynamics of the contrast and IMR, which is also derived from the CFD models. Results demonstrate that the computational CFD model effectively simulates the process of iodine contrast injection and yields meaningful computational angiography data. Furthermore, the data-driven framework presents a non-invasive, rapid, and accurate approach for IMR assessment.

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Isogeometric methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PRECONDITIONED B-SPLINE-BASED FINITE ELEMENT METHOD WITH UNFITTED MESHES FOR KIRCHHOFF PLATE

Han Yang[1], Wenquan Yuan[1], Chenguang Li[1], Fanke Wu[1] and Zhijun Liu[1]*

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ABSTRACT

B-splines are gaining popularity in finite-element approximations for solving fourth-order systems, such as Kirchhoff plate bending problems. This is due to their ability to not only provide exact geometric representations of curved domains (similar to the isogeometric concept) but also achieve higher global continuity with relative ease. However, the standard B-splines can only be constructed on Cartesian grids, which causes mesh cutting for complex domains and difficulties in imposing the Dirichlet boundary condition. Furthermore, difficulty in constructing high-quality mesh for complex domains facilitates the use of unfitted meshes. Unfitted finite element methods (FEMs) have been widely applied to second-order partial differential equations (PDEs), but their applications for fourth-order PDEs are rare. In this paper, we propose an unfitted FEM based on B-splines for the Kirchhoff plate problem, which is a typical fourth-order problem. A preconditioner based on global normalization and local Gram–Schmidt orthogonalization of bases is used to eliminate the ill-conditioning induced by mesh cutting. Besides, trimmed surface analysis is employed for the curved boundaries accurately.

The overall performance of the proposed methodology was evaluated through detailed numerical experiments of biharmonic equations and Kirchhoff plate bending problems. The methodology demonstrated excellent accuracy and optimal convergence. The proposed preconditioner effectively suppresses the ill-conditioning caused by the extreme cut and keeps the conditioning number at a very low level stably. The result demonstrates that the conditioning numbers and accuracies are approximately independent of how the mesh is cut by the model.

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Topology optimization for additively manufactured metamaterials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN INTEGRATED TOPOLOGY AND TOPOGRAPHY OPTIMIZATION FRAMEWORK FOR BUCKLING PERFORMANCE ENHANCEMENT OF THIN-WALLED STIFFENED STRUCTURES

Haotian Yang[*1], Renjing Gao[1] and Shutian Liu[1]*

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ABSTRACT

For thin-walled structures widely used in industry, external pressure and axial compression are common load cases and buckling is a key design consideration. The traditional method improves structural stability by designing stiffeners, but neglects their stiffness. Therefore, an integrated optimization design approach for base surface and stiffeners of thin-walled structures under uniform external pressure and axial compression is presented to improve stiffness and stability in this paper. In the first step, the Non-Uniform Rational B-Spline (NURBS) technique is used to parameterize the base surface, and then the control parameters are used as variables to change the shape of the base surface. In the second step, the Heaviside-function based Directional Growth Topology Parameterization (H-DGTP) is utilized to simultaneously optimize the layout and height of the stiffeners. In addition, the buckling load factors are computed by linearized buckling analysis, the lower bound of which is constrained to ensure the structural stability. By solving the optimization problem, the shape of base surface and the design of the stiffeners can reach a desirable match such that the structural stability is ensured and the stiffness is also optimized. The effectiveness of the proposed approach is demonstrated with numerical examples.

Battery modeling and computation: From material to device
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ELECTRO-CHEMO-MECHANICAL DEGRADATION OF NCM CATHODE MATERIALS: FROM POLYCRYSTAL TO SINGLE CRYSTAL

Hui Yang[*1]*

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ABSTRACT

Ni-rich transition metal layered oxides (NCMs) have been identified as the promising lithium-ion batteries (LIBs) cathode materials for their high reversible capacity. However, during electrochemical cycling, NCMs always suffer from fast structural degradation, leading to the inevitable performance fading of LIBs, which severely restricts their large-scale practical applications. Understanding the underlying mechanism of structural degradation is critical for the successful design of NCM structures with significantly enhanced cycling stability. Herein, an electro-chemo-mechanical model is developed to investigate the lithiation/delithiation cycling behaviors of both polycrystalline and single crystalline NCM cathode materials, including phase transformation, morphological change, stress generation, and damage evolution, based on which the underlying failure mechanism is uncovered. The new insight gained by this study is further adopted to guide the construction of NCMs from the aspect of surface modification to structural design, effectively promoting their cycling performance.

Advance and application of meshfree methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A TIME-DEPENDENT COLLOCATION FRAMEWORK FOR MULTI-PHASE COUPLING PROBLEMS WITH GEOMETRY EFFECTS

Judy Yang[*1] and I-Ting Liao*[1]

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ABSTRACT

In this work, a collocation framework is proposed for incremental-iterative analysis of double-diffusive natural convection problems in a porous enclosure on the basis of reproducing kernel collocation method. To untangle the nonlinear coupling problems, the forward difference method and Newton-Raphson method are adopted for temporal discretization and iteration, respectively. For verification purpose, the average Nusselt and Sherwood numbers are computed and compared with the reference solutions in the literature. The robustness of the proposed framework is demonstrated through solving various double-diffusive natural convection problems with satisfactory accuracy and efficiency.

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Scientific machine learning for geophysical applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HYBRID BI-LEVEL FILTERING METHODS FOR INVERSE PROBLEM AND DATA ASSIMILATION IN GEOPHYSICAL APPLICATIONS

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ABSTRACT

Bayesian inverse problems and data assimilation are prevalent in various applications, including subsurface modeling and weather data assimilation. Traditional statistical approaches, such as the Markov Chain Monte Carlo (MCMC), Ensemble Kalman Filter (EnKF), and Particle Filter, have been very successful in solving such problems but are often computationally expensive due to the repeated sampling of high-fidelity forward solvers. Alternatively, deterministic approaches also incur high computational costs as they require repeated solutions of the forward model and additional costs for solving adjoint models for gradient in the optimization loop. Recent advancements in deep learning-based surrogate models, such as DeepONet and Fourier Neural Operator, have demonstrated potential in significantly accelerating the solving of inverse and data assimilation problems. However, these pure data-driven approaches often fail to conserve physical quantities due to the absence of physical information. Although models like Physics-Informed Neural Networks attempt to address this issue, they are challenging to train and do not guarantee physical conservation, especially for complex problems with multiple data and physical constraints.

To better incorporate physical information in a different approach while using AI models, we proposed a hybrid bi-level MCMC approach to accelerate the solving of Bayesian inverse problem with accuracy comparable to pure numerical results. In this talk, we will first review some recent AI surrogate models for geophysical applications such as subsurface model and weather forecast. Then with the consideration of utilizing these advanced yet imperfect AI surrogate models, we will present the theoretical and computational framework of hybrid bi-level MCMC method and also extend the hybrid approach to the filtering methods such as EnKF and particle filter. In essence, we run two parallel MCMC chain or two level of filter algorithm with both AI surrogate model and numerical model. The GPU-accelerated AI surrogate model will run a long primary MCMC chain with a large number of samples, thereby reducing sampling error. And another shorter chain with much less numerical samples will correct the bias error from the primary MCMC chain with non-physical conserved AI surrogate model. We will demonstrate our approach through numerical experiments on some canonical mathematical examples as well as applications of bi-level filtering methods (EnKF and Particle filter) to simplified subsurface models, weather prediction models. In conclusion our hybrid methods allows the usage of current state of art AI models for practical application prior more robust physics informed machine learning methods become available.

Numerical modeling of granular and multiphase flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMPROVEMENT OF PREDICTIVE ACCURACY FOR REDUCED ORDER MODEL IN APPLICATION OF EULERIAN-LAGRANGIAN SIMULATIONS USING POSTERIOR ERROR ESTIMATION

Kai-en Yang[*1], Shuo Li[1], Guangtao Duan[1] and Mikio Sakai[1]*

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ABSTRACT

Multi-phase flows involving solid particles are widely studied by Eulerian-Lagrangian (E-L) simulations. Conventionally, such simulations are usually performed by discrete element methods coupled computational fluid dynamics (DEM-CFD). However, its applications easily suffer from high computational cost due to the huge amount of particles and complex physical equations.
Recently, with the advancements in data-science, development of surrogate model (SM) is extensively studied in numerical simulations for its advantage of high computational speed. It holds significant potential to tackle the computational cost challenge. One standing-out SM is the reduced order model (ROM). It is a typical SM that simplifies the original model mathematically through dynamics identification techniques such as proper orthogonal decomposition (POD). Previously, the preliminary adequacy and applicability of ROM on reconstructing granular systems with fluid-solid flows have been reported [1-2].

However, how to improve the predictive accuracy of SM on granular systems with violent fluid-solid flows remains unknown and challenging [3]. This is due to the lack of consistency between the high-fidelity model and SM caused by insufficient training data. As a result, the predictive accuracy can be easily deteriorated. This necessitates trial-and-error processes to find sufficient training data, which hinders the industrial applications.

To address this issue, this study newly reveals a finding that the data density is a key to improve the predictive accuracy through a posteriori error estimation. Sequentially, a novel technique for deciding the data density of SM is proposed. Specifically, a feasibility index is proposed to anticipate the predictive accuracy. Consequently, it is demonstrated that when the training data density is determined under proposed feasibility index > 2, the consistency of granular dynamics between SM and high-fidelity model can be guaranteed. Employed in the standing-out SM, reduced order model (ROM) for a bead mill simulation, this technique enables the successful decision of sufficient training data, resulting in the remarkable predictability (relative error < 5%) with an acceleration more than 1500 times compared to DEM-CFD. This technique offers a new approach to improve the predictive accuracy for SMs in applications of E-L simulations without trial-and-error.

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Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTISCALE MODELING OF SEISMIC WAVE PROPAGATION UNDER MULTIDIRECTIONAL SHAKING

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ABSTRACT

Nonlinear deformation analysis of seismic site response under multidirectional shaking requires representative constitutive models that accurately capture the intricate material behavior characteristics of such complex shearing conditions. This poses a significant challenge for existing advanced sand constitutive models, which are often formulated, developed, and refined based on laboratory experiments involving unidirectional cyclic shearing. While continuous refinement of these constitutive models to address the complexities of multidirectional shaking is possible, the discrete element method (DEM) provides an alternative approach to bypass such extensive efforts. Particle assemblies prepared by DEM effectively encapsulate the crucial aspects of the response of granular materials under multidirectional loading.

This study develops a multiscale modeling framework that hierarchically couples a global-scale finite element method (FEM) for resolving hydromechanical feedback with a local-scale DEM solver, which can adequately replicate the sand deformation response under dynamic loading. This approach addresses the modeling challenges of sand deposits subjected to multidirectional shaking. The effectiveness of this framework is first evaluated by simulating benchmark examples, including 1D consolidation and cyclic simple shear tests. This framework is then validated by modeling centrifuge experiments that involve the dynamic response of a soil column under both uni- and multidirectional shaking. The simulations reveal the more detrimental effects of multidirectional shaking, including the accumulation of higher excess pore pressure and induction of larger settlement, compared to unidirectional shaking. The simulation results are also compared with experimental measurements, including acceleration history, spectral response, excess pore water pressure development, and subsequent vertical settlement. These comparisons demonstrate the capability and reliability of the multiscale modeling framework in accurately capturing the complex behavior of sand deposits under multidirectional shaking.

Multi-physics multi-scale numerical simulation and machine learning based modelling for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A THERMODYNAMICALLY CONSISTENT PHASE-FIELD-MICROMECHANICS MODEL OF MICROSTRUCTURE EVOLUTION IN SINTERING-BASED ADDITIVE MANUFACTURING

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ABSTRACT

Sintering is a pivotal technology for processing ceramic and metallic powders into solid objects in additive manufacturing. A profound understanding of microstructure evolution during sintering is essential for manufacturing products with tailored properties. While various phase-field models have been proposed to simulate microstructure evolution in solid-state sintering, correctly incorporating the densification assumption—where particles move toward each other by rigid body motion—remains a challenge.

The fundamental obstacle lies in the ad hoc treatment of particle motion, where the thermodynamical driving force cannot be derived from the system's free energy. In this work, we present a novel phase-field-micromechanics model for sintering. We relax the rigid body assumption, allowing powder particles to mechanically deform through surface and grain-boundary tensions. Subsequently, a unified energy law is defined, and the governing equations for microstructure evolution in sintering are derived using variational principles.

Our approach ensures thermodynamic consistency, with the driving force for particle motion derived from the system's free energy. Consequently, the proposed phase-field-micromechanics model guarantees the evolution of microstructure in a direction that reduces the system's energy. We rigorously validate this model against recent benchmarks of theoretical analysis.

Design and mechanics of mutifunctional composites and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODE-SWITCHING METAMATERIALS ACHIEVING ASYMMETRIC, NON-RECIPROCAL, AND ADJUSTABLE POISSON'S RATIOS THAT BREAKS THERMODYNAMIC LIMITS

Qingsheng Yang[*1] and Aijie Tang*[1]

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ABSTRACT

While metamaterials with unconventional Poisson's ratios have been extensively explored for their counterintuitive and desirable properties, most exhibit only a single behavior. Here, we design novel metamaterials capable of both positive and negative Poisson's ratios, which simultaneously demonstrate outstanding performances: asymmetric, non-reciprocal, and even exceeding thermodynamic limits. These abnormal properties are achieved by combining honeycomb and re-entrant structures with self-contacting stops set at different positions. The unique topology allows for mode switching, where the unit cell can transition between "honeycomb" and "re-entrant" configurations under different load conditions. This mode convertibility endows the metamaterials not only different signs of Poisson's ratios under various load conditions in a single direction but also anisotropy in orthogonal directions. Through theoretical analysis, the deformation modes and the corresponding Poisson's ratios are predicted. Experiments and simulations then validate the intriguing Poisson's ratios and the model predictions. Notably, these Poisson's ratios can be further tailored by adjusting the initial states of the self-contacting stops, offering a powerful tool for manipulating Poisson's ratios and unlocking new functionalities of metamaterials.

Multiscale computational and data-driven approach of advanced materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MESOSCALE STUDY OF POLYMER PYROLYSIS USING COARSE-GRAINED MOLECULAR DYNAMICS SIMULATIONS

Vinh Phu Nguyen[1], Inseok Jeon[1], Seunghwa Yang[1] and Seung Tae Choi[1]*

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ABSTRACT

A deep understanding of how polymeric materials break down under heat is crucial for designing effective thermal protection systems. However, gaining this understanding involves grappling with complex phenomena that occur at various spatial and temporal scales. To bridge the gap between the many detailed simulations and broader modeling approaches in existing literature, we undertake an innovative mesoscale investigation of the pyrolysis process using coarse-grained molecular dynamics (CG MD) simulations. In this study, we use atomically bonded polyethylene (PE) with implicit hydrogen as a representative model for polymers. The changes in PE composition during thermal decomposition are modeled by incorporating bond-breaking phenomena based on either bond energy or bond length criteria. To refine the protocol for bond dissociation, cook-off simulations are implemented to compare reaction products with ReaxFF simulations. This approach extends to simulating aerobic high-thermal pyrolysis under extensive oxygen bombardment on a nanoscale. This allows us to observe intricate phenomena occurring from the material's surface to its depths. Mesoscale simulations effectively predict the intrinsic thermal durability of model polymers under extreme conditions, regardless of the presence or absence of an oxygen environment. These predictions provide crucial thermal degradation characteristics necessary for broader-scale degradation and removal simulations. This work represents an initial exploration into understanding polymer pyrolysis at the mesoscale, contributing to a deeper comprehension of the concept on a larger scale.

Contact and interface mechanics: Modeling and computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN IMMERSED BOUNDARY APPROACH FOR FLUID-STRUCTURE INTERACTION SIMULATION USING THE MATERIAL POINT METHOD

Wen-Chia Yang[1] and Yu-Ting Lin*[1]

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ABSTRACT

The Material Point Method (MPM) has proven effective in modeling large deformation scenarios and in tackling complex fluid-structure interaction challenges. This method is potentially a valuable tool for understanding structural behavior during extreme events such as tsunamis, flash floods, and debris flows. In these scenarios, the dimensions of structural components, like beams and columns, are often significantly smaller than the computational domain, leading to inaccuracies in stress distribution within particle-represented structural elements when grids are sized according to the domain scale. To address this, Yang's (2016) immersed boundary approach for MPM is extended into a contact algorithm between beam-column elements and MPM computational grids. It treats beam-column elements as velocity boundary conditions during grid evolution phases and updates these elements during the particle updating phases. This algorithm integrates smoothly into the MPM framework with minimal changes to existing MPM codes. The presentation will explore the procedures of this contact algorithm in MPM with beam-column elements, its validation through two-dimensional simulations involving frictional sliding and impact loads on beams, and conclude with a demonstration of a complex two-dimensional water-structure interaction problem, showcasing the algorithm's capabilities.

Lattice Boltzmann modelling and study of complex flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL SIMULATION FOR THE REACTIVE MULTIPHASE FLOW IN POROUS MEDIA DURING THE CARBON CAPTURE AND STORAGE PROCESS

Wenxin Yang[*1], Hai Sun[1], Lei Zhang[1], Dongyan Fan[1], Shuaishi Fu[1], Junjie Zhong[1] and Jun Yao[1]*

[1]*China University of Petroleum*

ABSTRACT

In recent years, the extensive using of fossil fuels has led to a substantial release of greenhouse gases, resulting in a pronounced warming trend in the Earth's climate. To mitigate the process of global climate warming, Carbon Capture, Utilization, and Storage (CCUS) projects have gained prominence, with the efficient sequestration of CO2 into geological formations becoming a focal concern. In the process of CO2 sequestration, the permeation behavior of CO2 in water crucially determines its storage capacity and rate. On the one hand, the dissolution of CO2 in water increases the storage capacity. On the other hand, some rocks in the formation, such as glauberite, will dissolve under the combined action of carbon dioxide and water, thereby increasing the storage space of carbon dioxide. To comprehensively investigate the various influencing mechanisms in the CO2 sequestration process, pore-scale simulations offer an effective approach, allowing for a microscopic examination of mechanisms and a systematic analysis of influencing factors to further guide the sequestration of CO2. The lattice Boltzmann method, as a mesoscale approach, efficiently facilitates multiphase and multiscale coupling, enabling the treatment of complex solid-liquid/gas-solid boundary conditions. Thus, in this study, the lattice Boltzmann method was adopted for research purposes.

In this study, a new LB model was built to consider the effect of both CO2 dissolution in water and salt dissolution mechanisms on the CO2 storage process. What’s more, the CST-LB model was adopted to describe the interfacial mass transfer, and the VOP method was used to update the structure of porous media. The impacts of factors such as wettability, salt concentration, and porosity on the CO2 sequestration process were comprehensively explored. The results indicate that, during the displacement and dissolution processes of CO2 in the aqueous phase, an increase in CO2 concentration in water leads to the gradual dissolution of some soluble salts in the solid phase. But there are some risks. While this expands the storage space for CO2, the dissolution of soluble salts results in the phenomenon of breakthrough points between CO2 and water, forming preferential channels that cause a substantial outflow of CO2. Additionally, when the wettability angle of the rock phase is greater, after CO2 displacement, some water remains in the porous medium, reducing the CO2 storage space and consequently diminishing sequestration capacity. This study provides crucial guidance for the sequestration of CO2.

Uncertainty quantification and scientific machine learning for predictive modeling of complex systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NEW PARADIGM FOR UNCERTAINTY QUANTIFICATION USING THE KOOPMAN OPERATOR

Bian Li[1], Yi-An Ma[2], Nathan Kutz[3] and Xiu Yang[*1]*

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[3]University of Washington

ABSTRACT

We propose a new uncertainty quantification (UQ) framework for dynamical systems with random parameters. Unlike conventional UQ approaches in which a set of basis functions associated with random variables are used to construct a surrogate model of the quantity of interest (QoI), our new method uses the eigenfunction and eigenvalues of the Koopman operator of the system to construct the surrogate. The advantage of this new approach is that the eigenpairs of the Koopman operator incorporate key features of the dynamics, hence it can be more efficient in capturing behavior of the system. Empirically, our approach exhibits exponential convergence if the solution is smooth. The approach does not use time integration algorithms like the Runge-Kutta scheme as the statistics of the QoI relies on the moment-generating function of the random variable in the system. In addition to this intrusive approach, we will present a non-intrusive method that is compatible with most sampling strategies from Monte Carlo simulation to probability collocation method. This non-intrusive method reuses the computed eigenfunctions and eigenvalues of the underlying system's Koopman operator to reduce the computational cost dramatically. Moreover, for stochastic dynamical systems with additive noise like stochastic differential equations, our approach can directly evolve moments, which helps to evaluate the system's statistics, e.g., mean, variance, skewness, efficiently. Finally, our algorithms enable parallelization for solving dynamical systems with or without uncertainties from a new perspective. We will demonstrate the accuracy and efficiency of our new methods using ordinary and partial differential equations.

Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RESIDUAL STRESS PREDICTION IN LPBF USING A FINITE VOLUME METHOD BASED COUPLING FRAMEWORK

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ABSTRACT

Residual stress generated in laser powder bed fusion (LPBF) process is a key factor impairing the integrity and reliability of additively manufactured engineering structures. This work proposed a novel finite volume method-based coupling framework to predict the integrated thermal-fluid-metallurgical-mechanical behaviors during LPBF process. The framework directly unifies the high-resolution fluid flow and solid deformation/stress simulations in LPBF, which enables the fast residual stress simulation at track scale, and facilitates a thorough investigation into the effects of microstructures and solidified geometry profiles on residual stress fields. Various operating conditions including single-track, multi-track and multi-layer were simulated to explore the spatiotemporal variations of thermal stress and final residual stress fields. And the influences of solid-state phase transformation and pores defects were clarified. The metallographic and the nanoindentation experiments were separately carried out on the well-crafted samples to evaluate the microstructure and RS fields. Comparisons between the simulations and experiments demonstrated a dependable similarity, which validates the effectiveness of established framework for full-process and multi-physics modeling of LPBF. The findings of this work will enhance the comprehension of RS origination and offer practical instructions for RS prevention in the LPBF manufacturing.

INVERSE PROBLEM PREDICTION BY USING THE BEM AND DNN

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ABSTRACT

An approach for solving the inverse problem of computational mechanics is developed by the data driven algorithm in conjunction with model driven method based on BEM. The inverse problem is formulated as a regression problem, which extracts the solution of highest probability through machine learning (ML) from a large amount of data. The efficiency and accuracy of data generation is guaranteed by using the BEM, which also actualizes the data compression by means of dimensionality reduction. The efficiency of this approach is illustrated by two examples. First, five-step damage identification including damage detection, location, classification, extent and prediction is carried out. The boundary strains of the forced structures are collected by the elastostatic BEM, which is also easy to collected though the strain gauge sensors settled on the boundaries of the monitored structures. A series connection neural network algorithm composed of classification and regression NN models is established to accomplish complete 5-stage damage identification. Next, acoustic localization is presented. Acoustic pressure on microphone array and source plane is analyzed by the acoustic radiation BEM. The mapping relationship is constructed by a CNN model. A high precision about 99% can be achieved for both of two examples by the present algorithm and which is also feasibility to apply in the actual structural health monitoring and acoustic localization.

Recent advances in meshfree and particle methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A NEW COMPUTATIONAL FRAMEWORK OF FPM BASED ON MATRIX DECOUPLING

Yang Yang[*1], Xu Fei[1] and Li Yaoyu[1]*

[1]*Northwestern Polytechnical University*

ABSTRACT

Finite Particle Method (FPM) is a significant improvement to the traditional SPH method, which could effectively improve the accuracy in the interface or the boundary region. In traditional FPM format, the numerical iteration scheme for solving higher order derivatives was creatively transformed into the calculation of the derivatives simultaneously through linear equations, while the resulting long computational time has become a major obstacle to its development. In this paper, a new computational framework of FPM was proposed based on matrix ecoupling, in which the kernel function information, the particle distribution information and the function information could be clearly decoupled. Based on this framework, some new FPM improvement formats and their derived combination formats were proposed under different assumptions, and then were successfully applied to some typical numerical examples.

Complex fluid flows in engineering: Modeling, simulation, and optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CURING INSTABILITY ON INTERFACE TRACKING UTILIZING WEAKLY IMPOSED DIRICHLET CONDITIONS

Yundong Yang[*1] and Jaewook Nam*[1]

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ABSTRACT

Understanding the behavior of interfaces in engineering processes involving fluids is crucial. One such industry is secondary battery manufacturing, which utilizes the coating process. Numerical computation is used to reproduce the interface in this process, which includes a liquid-gas interface with a high aspect ratio, presenting several challenges.

One of the main challenges is the instability of the liquid-gas interface caused by oscillatory behavior along the computational domain. Fluctuations in the pressure field generate wiggles in the interface, which amplify over time. This instability resembles the "checkerboard mode" observed in various flow simulations [1].

The instability occurs when the Dirichlet condition excessively restricts the degree of freedom of interfacial nodal displacement. The interface tracking technique requires a no-penetration condition for the liquid-gas interface, restricting only the displacement in the surface's normal direction. However, additional conditions that limit the tangential direction are commonly used for computational convenience.

A method that weakly imposes the Dirichlet condition, such as Nitsche's method, is commonly used to address this issue in remeshing including the elastic mesh update method [2]. Nitsche's method retains the advantages of Lagrange multiplier and penalty methods, providing variational consistency and a symmetric linear system.

This study modifies Nitsche's method by restricting only the normal direction with a penalty term. It aims to investigate the impact of this relaxation of restrictions on the transient behavior and instability of the interface using a 2D model problem that incorporates the aspect ratio and characteristics of the coating process. The study also aims to empirically determine the influence of the penalty parameter and select the optimal value. The findings of this study could provide insights into the behavior of liquid-gas interfaces and contribute to stable interface simulations in various processes.

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Machine learning and multiscale modeling for complex materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREDICTION OF STRUCTURE-PROPERTY LINKAGES IN HIGHLY PARTICLE-FILLED POLYMER COMPOSITES UNDER VARIOUS STRAIN RATES AND TEMPERATURES USING THE MACHINE LEARNING

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ABSTRACT

In the study of highly particle-filled polymer composites (HPFPCs), the complexity of their microstructure makes it difficult to predict their mechanical properties using standard numerical calculation methods. This study employs machine learning techniques to effectively predict the effective mechanical properties of HPFPCs under various microstructures, such as effective elastic modulus and peak strength. The initial step in the study was the design and establishment of a relevant dataset for HPFPCs, which is crucial for assessing the role of machine learning. To create a comprehensive and effective dataset, the research involved analyzing Scanning Electron Microscope (SEM) images, from which we can extract the dispersion of particles within HPFPCs, including details about particle size, distribution, and volume fractions. Additionally, mechanical parameters were obtained using our in-house nonlinear finite element numerical framework. Subsequently, several neural network models were designed and implemented specifically for this problem. Utilizing our established training set, these neural network models were trained and tested. The study conducted a comparative analysis to evaluate the effectiveness of different neural network models in predicting the material structure-property relationships of HPFPCs under varying strain rates and temperatures. Furthermore, the research explored how hyperparameters in the neural network models, such as activation functions, loss functions, and structural hyperparameters, affect the prediction accuracy. The findings indicate that neural network models, particularly those based on image recognition technology, are highly effective in revealing the mechanical properties of HPFPCs. Our work explored the combining advanced machine learning with traditional analysis to predict the mechanical properties of HPFPCs. As to the future work, by designing and building a new comprehensive dataset, we can extend the HPFPCs problem to more advanced machine learning models like Vision Transformers. Meanwhile, we aim to automate our hyperparameter tuning process, which could be applicable to other similar machine learning problems in material science.

A ROM-ACCELERATED ENSEMBLE TRANSFORM FILTER FOR DATA ASSIMILATION OF NONLINEAR DYNAMICAL SYSTEMS

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ABSTRACT

We present an ensemble transform filter (EnTF) accelerated by hyperreduced-order models (HROMs) to enable rapid and reliable data assimilation of large-scale dynamical systems that exhibit strong nonlinearities. The filter estimates the state of the system using a mathematical model based on nonlinear unsteady partial differential equations (PDEs) and noisy, sparse observations. Our formulation builds on two key ingredients. The first is the EnTF [1], which generalizes the standard ensemble Kalman filter (EnKF) to stronger nonlinearities by constructing a nonlinear transport map between the filtering and analysis distributions. However, the EnTF scales poorly with the state dimension and requires a large state ensemble, which renders it cost prohibitive for large-scale PDE-governed dynamical systems. To overcome this computational challenge, we introduce the second key ingredient: HROMs constructed using proper orthogonal decomposition and the empirical quadrature procedure [2]. The HROMs (i) significantly reduce the state dimension, which mitigates the scaling issue of the transport map, and (ii) reduce the cost of ensemble simulation in the forecast step, which enables the use of a larger ensemble. Moreover, we analyze the stability issue that arises when EnTF is applied to HROMs that use a modal state representation, and devise a strategy to stabilize the filter. We apply the filter to unsteady, compressible, separated flow over an airfoil in the presence of synthetic velocimetry data. We demonstrate that the combination of the EnTF and HROM enables nonlinear filtering of the PDE-governed dynamical system, and assess the efficacy of the nonlinear EnTF relative to the standard EnKF.

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Modeling friction and wear
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

WEAR ANALYSIS AND OPTIMIZATION DESIGN OF THE ROPE SHEAVE WHEEL MECHANISM

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ABSTRACT

With the continuous improvement of modern transmission equipment, lifting mechanism has been widely used, among which the rope sheave lifting mechanism because of its small size, strong closing, high transmission efficiency, high timeliness, convenient and other characteristics, is widely used in high-altitude operation combat, building inspection and maintenance and life transportation and other important fields.However, the rope sheave structure is still designed based on experience and experimental test results. There is little research on the mechanical properties between the flexible rope and the rope sheave and the composite wear of the rope. Therefore, this paper builds a mathematical model of static rope composite wear based on the basic wear law,and optimize the flexible rope sheave wheel lifting mechanism.Firstly, the nonlinear equations with single objective and multiple parameters are established by mathematical model, and the structural parameters of rope sheave wheel are designed by ASA algorithm to minimize the compound wear of static rope.Secondly, based on the optimization design of rope sheave wheel system performance, the multi-objective equations of lifting force, composite wear and rope sheave wheel structure parameters are established. NSGA-Ⅱ algorithm is used to optimize the design of rope sheave wheel structure parameters, so that the static rope compound wear is minimized and the rope wheel system performance is optimized.It provides theoretical guidance and design basis for more precise application of flexible rope sheave wheel lifting mechanism.

Advanced materials and smart structures: Modeling, simulation and testing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTI-OBJECTIVE OPTIMIZATION OF PIEZOELECTRIC ENERGY HARVESTERS FOR POWER GENERATION AND SENSING IN STRUCTURAL HEALTH MONITORING

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ABSTRACT

As infrastructure such as bridges plays an increasingly important role in social operations, structural health monitoring (SHM) implemented by wireless sensing devices has become the main way to protect human safety and property. However, long-term and real-time data transmission poses challenges for the energy supply of sensors. Piezoelectric energy harvesters (PEHs), as green devices capable of harvesting universal and stable mechanical vibrations, have the potential to address the constraints of unsustainable energy supply in SHMs. On the other hand, piezoelectric materials are commonly used as actuators and sensors to provide sensing functions, but the energy-harvesting effect of piezoelectric materials has been ignored. Therefore, this study explores the multifunctional integration of PEHs, combining energy supply and sensing. PEHs are modelled as cantilever structures based on Kirchhoff-Love plate theory and Isogeometric Analysis (IGA) to obtain accurate and efficient simulation results. In addition, the sensing process aimed at detecting bridge damage is based on the voltage signal generated by PEHs during energy harvesting. Then the Wavelet Synchro-squeezed transform (WSST) is applied to obtain damage features after the pre-processing of the voltage signal. Moreover, WSST images are used as the input of an unsupervised learning algorithm, namely convolutional variational autoencoders (CVAE), for label-free training and identification of bridge damage severity and location. It is worth mentioning that both the simulated signals from the vehicle-bridge interaction (VBI) model and collected signals from a real bridge in Australia are employed to demonstrate the practicability of this study in actual engineering. In order to further improve the sensing and energy harvesting capabilities of PEHs, the shape optimization based on the Particle Swarm Optimization (PSO) algorithm retrieves the optimal geometric configuration under multi-objectives, achieving the optimal self-powered sensing system based on PEHs.

The phase field method for fracture: Theory, numerics, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A CHEMO-MECHANICAL COUPLED PHASE FIELD MODEL FOR STRESS CORROSION CRACKING

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ABSTRACT

A thermodynamically consistent framework for chemo-mechanical-fracture coupled model is presented in this contribution to simulate the stress corrosion cracking (SCC) process. The film rupture mechanism is used to simulate SCC process, the dissolution process of the metallic material is governed by a diffusion-convection equation. To overcome the numerical oscillation problem stemmed from the standard Galerkin finite element procedure when convection term is in dominate, a streamline upwind Petrov-Galerkin (SUPG) finite element method is adopted in this work. The fracture process is simulated by using the facture phase field method, the degradation effects of corrosion on mechanical properties is considered and investigated. The proposed model is validated through several numerical simulation examples.

Probabilistic learning and constrained generative models for uncertainty quantification
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PROBABILISTIC MODELING AND SAMPLING OF CONSTITUTIVE LAWS FOR HYBRID COMPOSITE MATERIALS USING PROBABILISTIC LEARNING ON MANIFOLDS

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ABSTRACT

In this paper we describe the application of Probabilistic Learning on Manifolds for constructing constitutive laws for complex material systems. These laws can be synthesized either from a training dataset obtained either from experimental data or from a high-fidelity simulation that resolves sub scale details. This experimental dataset is used to synthesize a joint density function for tuples of stress, strain, microscope characteristics, and damage. For damage, we use both strain energy density as function of strain, and the toughness of the specimens. For microscale characteristics we use mechanical properties of fibers and resin.

Once the joint density function is constructed, conditioning on strain values produces the probability density function of stress values. Probabilistic scatter of these stress values is attributed to unobserved (unspecified) properties of micro-constituents and damage. Alternatively, by conditioning on fiber properties, the probability density function of damage quantities can be calculated. In this manner, sensitivity of probabilistic quantities of interest to any observable can be assessed.

Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMMERSED-BOUNDARY APPROACH BASED ON INTEGRATED RBFS AND SMOOTH EXTENSION FOR SOLVING PDES IN COMPLEX DOMAINS

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ABSTRACT

We propose an immersed-boundary approach, based on five-point integrated radial basis function (IRBF) stencils and smooth extension of the solution, for solving the two-dimensional elliptic partial differential equation (PDE) in a geometrically complex domain. The discretisation is simply based on a rectangular Cartesian grid, which does not conform to the geometry of the domain. High-order accuracy is achieved by including nodal derivative values in local IRBF approximations, and forcing the solution to be globally smooth in the entire encompassing domain. In solving for the smooth extension of the solution, the constants arising from the process of integrating the RBFs are utilised to include the boundary values of the derivatives in the IRBF approximations, which enables high-order PDEs in the extension domain to be enforced at every interior node. Numerical experiments will demonstrate that the approach provides a simple, efficient and high-order immersed boundary scheme which can solve problems with smooth and non-smooth boundaries.

Towards predictive digital twins: Innovative algorithms for physics-, data-assisted and hybrid modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT OF AN EXTENDED CHEMICAL REACTOR NEURAL NETWORK FOR MODELING REACTORS WITH TIME-VARYING TEMPERATURE

Katleya Medrano[1], Tatsurou Yashiki[1], Mutsuki Koga[2], Naoki Hosoda[2], Yohei Yamaguchi[2], Atsuya Shimokawa[2], Ryuichi Suzuki[2], Ryoichi Aikawa[2] and Kunugi Kondo[2]*

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ABSTRACT

We are developing a simulator technology for chemical reactors that leverages both data and domain knowledge. Conventionally, reactor simulation uses pure physics-based models which can be challenging to build when the reactions involved have complex or unknown kinetics. Meanwhile, recent works based on data-driven approaches can only generate black box models which do not give insight on actual reaction pathways.

Against this background, we adopted a data-driven model that uses differential equations for chemical reactors called “Chemical reaction neural network” (CRNN) [1]. The CRNN was designed to follow basic physical laws, such as the law of mass action and Arrhenius law, generating an explainable data-driven model. It discovers kinetic models and predicts concentrations; however, its scope is limited to constant-temperature reactors.

In this study, we propose a dynamic temperature CRNN (DT-CRNN) which extends the application of the original CRNN to reactors with dynamic temperature. In this extension, instead of forcing a constant temperature output data as in the previous approach, we add time-series temperature as input data to the neural network calculation. We specifically feed temperature data in the evaluation step of the neural network as ordinary differential equations. In this way, the DT- CRNN captures the underlying behavior of reactor temperature while maintaining the simple architecture of the original CRNN. We specifically study a hypothetical batch reactor equipped with a temperature control system for two irreversible and exothermic reactions as target reactor to evaluate the proposed DT-CRNN [2].

Results show that DT-CRNN could closely approximate the reaction equations of the target reactor. The kinetic parameters were also estimated within 2% error. Moreover, the accuracy of the simulated concentrations did not drastically change when the measured concentration data for training was reduced from every 1min to every 60min. Overall, results suggest the effectiveness of the DT-CRNN for building reactor models even with time-varying temperature data and limited concentration measurements. Combining the DT-CRNN with a temperature prediction model is left as future work.

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Contact and interface mechanics: Modeling and computation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELS AND METHODS FOR CONTACT MECHANICS AT THE ROUGHNESS SCALE

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ABSTRACT

In the modeling and simulation of numerous engineering systems involving contact, friction, wear, and lubrication, surfaces are often assumed to be smooth and well-described by the associated CAD models. However, in some particular cases, surface roughness must be taken into account, either through a special constitutive interface model or in a more explicit manner. In either case, both for constructing relevant constitutive tribological models and for direct numerical simulation, it is necessary to properly characterize surface roughness and incorporate it into computational models. At the same time, it is important to use material and friction models relevant to the considered scale. The complexity of the arising problems stems from the multiscale nature of roughness, the lack of scale separation, and the necessity to handle the problem in three-dimensional space.

In this talk, we will provide a brief overview of the available methods, including the FEM (finite element method) and the BEM (boundary element method) in classical, FFT, and fast-BEM formulations constructed on hierarchical or H-matrix concepts. Additionally, we will present a combined FEM/BEM approach that enables handling the contact problem in a non-intrusive way, as an auxiliary one. Some examples of multiphysical coupling strategies for thermo-electro-mechanical contact problems will be demonstrated.

Apart from the methodological aspects, we will discuss models capable of accounting for the effect of roughness on the evolution of the true contact area, static friction, electrical and thermal conductivity, and fluid transmissivity. The presentation will conclude with a discussion on the future challenges and opportunities in the field.

FROM VEHICLE BRIDGE INTERACTION TO VEHICLE-SCANNING METHOD FOR BRIDGE MONITORING

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ABSTRACT

Vehicle-Bridge Interaction (VBI) happens when a vehicle crosses a bridge, leading to vibrations in both the vehicle and the bridge [1]. The Vehicle-Scanning Method (VSM) [2] uses these vibrations to understand the bridge's condition. It's like using the vehicle as a moving sensor to pick up information about the bridge, such as its natural frequencies and mode shapes. From a theoretical analysis, VSM also simplifies VBI, making it easier to understand and interpret the interaction between the vehicle and the bridge. It separates the responses of the vehicle and the bridge, based on the idea that the vehicle's weight doesn't really affect the bridge's vibration. Compared to traditional bridge inspection methods, VSM has several benefits. It's cost-effective, doesn't disrupt traffic, can be used continuously, and can be easily scaled up. In short, VBI is a complex but interesting area of research with real-world applications for bridge engineering. It's the foundation for developing VSM, a promising way to monitor and assess the health of bridges. But we need more research to better understand and use VBI and VSM.

Acknowledgement
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AXISYMMETRIC VIRTUAL ELEMENTS

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ABSTRACT

Recent research extends the capabilities of the virtual element method (VEM) by introducing axisymmetric virtual elements. Axisymmetric virtual elements are achieved by modifying a 2D VEM formulation by augmenting the strain displacement matrix to include tangential strains. Mean value coordinates (MVC) are utilized to provide the required ingredients while still allowing for concave and convex elements. Element volume is properly accounted for by using the volume of revolution associated with each element. Axisymmetric problems of elasticity and plasticity are successfully solved and compared to benchmark problems. For certain classes of solid mechanics problems, the ability to use an axisymmetric virtual element is computationally more efficient than an otherwise required 3D discretization. Very good results are also demonstrated for problems of near incompressiblity. Results and future research directions are discussed at the conclusion of the presentation.

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Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DUCTILE FRACTURE ASSESSMENT IN TI-6AL-4V ALLOY FABRICATED BY ELECTRON BEAM MELTING (EBM)

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ABSTRACT

Additive Manufacturing (AM) has introduced in a new era of complex and optimized geometries, necessitating an in-depth exploration of the mechanical behavior of AM components. This research investigates into the Ti-6Al-4V alloy manufactured through Electron Beam Melting (EBM), as AM technique. Employing a hybrid experimental-numerical approach, the study focuses on evaluating and modeling Ductile Fracture (DF) under diverse loading conditions.

Three ductile fracture models, the Johnson-Cook (JC), Modified Mohr-Coulomb (MMC), and Hosford-Coulomb (HC) models, are employed to simulate fracture behavior. Simulations are developed using ABAQUS software. The JC model is available on software library, and the MMC and HC model were implemented through VUMAT subroutine. The JC model excels in compression cases, while the MMC and HC models demonstrate superior performance in positive triaxiality situations. Seeking a comprehensive model, an extended MMC model is proposed to predict fractures under both negative and positive triaxiality, displaying an average error of less than 7% when compared to experimental results. This modification introduces novel conditions, enhancing the model's applicability across a broader spectrum of scenarios.

This study advocates for the adoption of the proposed ductile fracture model, calibrated through experimental tests, as a robust tool for predicting fracture behavior in Ti-6Al-4V alloy components fabricated using EBM. The model's versatility is underscored by its ability to accurately capture fracture deformations across a range of loading conditions, providing valuable insights for optimizing AM processes.

Nanomechanics and nanoscale thermal transport for new materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NOVEL COMPUTATIONAL METHODS FOR THE MECHANICAL PROPERTY OF ULTRA-SOFT TWO-DIMENSIONAL MATERIALS

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ABSTRACT

The ultra-soft and ultra-thin features bring challenges for accurately evaluating the mechanical property of two-dimensional materials. In this work, we propose some novel computational method of the elastic modulus, shear modulus, Poisson's ratio and bending stiffness. The analytical atom-based molecular mechanics model is established to predict the elastic modulus, Poisson's ratio and shear modulus of the single-layer 2D transition-metal dioxides and dichalcogenides. This method is validated through the calculation of the mechanical property of Molybdenum disulfide (MoS2). The results indicate that the elastic modulus, Poisson's ratio and shear modulus of MoS2 with infinite size are 178.9 GPa, 0.22 and 73.3 GPa, respectively. We can observe the obvious dependence of the elastic modulus, Poisson's ratio and shear modulus on the chiral direction and characteristic size. Based on the constructed analytical method, we report a library composed of the mechanical properties of 34 types of 1H-MX2. It is found that the mechanical performances of 1H-MX2 depend on the period and group numbers of elements. The obtained results are in good agreement with the existing experimental and numerical results. Furthermore, the roles of molecular structure and force field on the mechanical properties are revealed, which is beneficial in predicting the mechanical performances of the potential and unreported 1H-MX2. For the bending stiffness, a coaxial spring-driven method is established, which exhibits great ability in the computation of the bending behavior for the ultrasoft two-dimensional materials. The findings offer an important theoretical basis for the reverse design and optimization of 1H-MX2 material-based nanodevices, nanochannel, etc., through nanostructure-property relationships. The supports from the National Natural Science Foundation of China (12372192, 11972108, 12072061, 12072062), the National Key R&D Program of China (2022YFB4201200) and Fundamental Research Funds for the Central Universities are gratefully acknowledged.

Design and mechanics of mutifunctional composites and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CONCURRENT OPTIMIZATION METHOD OF PRINCIPAL STRESS ORIENTATION INTERPOLATED CONTINUOUS FIBER ANGLE (PSO-CFAO) AND STRUCTURAL TOPOLOGY

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ABSTRACT

Abstract: Continuous fiber-reinforced polymers (CFRPs) have been widely applied in aerospace and other fields due to their excellent mechanical properties, and have become the best substitute for traditional metal materials. The designability of CFRP structural topology and fiber distributions provides an opportunity for achieving better physical properties through optimization. However, local optima and the dependence of initial fiber angle variables during optimization process make the concurrent optimization of fiber orientation and topology a challenging problem, which cannot exploit the full potential of CFRPs. In this paper, the principal stress orientation interpolated continuous fiber angle optimization (PSO-CFAO) method combined with the independent continuous mapping (ICM) method is proposed to realize the design of CFRP structures with a clear macroscopic topology and microscopic fiber distribution. A sigmoid function is applied to interpolate the fiber angle variables by the principal stress orientation. The fiber angle variables are modified and a continuous fiber design is obtained during the iteration process, which reduces the possibility of a local optimum. Numerical examples are provided to prove the effectiveness and stability of the proposed method, and the expected results are acquired for different initial fiber angles and mesh densities. The proposed method is effective to reduce the risk of local optima and can apply to the optimization problem with a large number of elements, which can provide guidance for the design of CFRP structures and the planning of fiber paths.
Key Words: Continuous fiber reinforced polymer, Topology optimization, Continuous fiber angle optimization, Principal stress orientation

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Advances in neural operators for scientific modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A SURROGATE MODEL FOR RAPID SOLUTION OF ACOUSTIC WAVE EQUATION BASED ON THE BOUNDARY ELEMENT METHOD AND FOURIER NEURAL OPERATORS

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ABSTRACT

A modern approach to control sound is through the development of sound-control materials/structures, which enable a wide range of applications such as noise reduction and non-contact particle manipulation. Designing these sound-controlling metamaterials requires accurate and efficient simulation methods for solving the unbounded acoustic wave equation with changing domain and frequencies. To facilitate the design optimization, surrogate models that are significantly more efficient than full-scale simulations are highly desirable. In this work, we present our recent work on the development of such surrogate models based on the concept of Fourier neural operators (FNO). FNO was originally developed to learn the mapping from a parametric space to the solution space for a family of partial differential equations within a finite domain (Li et al., 2020). However, for unbounded problems with changing domains, directly applying FNO is not feasible. Therefore, we propose to a method that combines the boundary element method (BEM) with FNO. The acoustic BEM offers advantages such as boundary discretization only and is particularly suitable for solving wave propagation problems in infinite domains. In our approach, we use FNO to construct a surrogate model that maps the boundary Euclidean space, representing the geometry of the sound-controlling structure, to the corresponding boundary solution space. Once the boundary values are known, the boundary integral equation is then applied to calculate the acoustic pressure at desired points within the infinite domain. To validate the performance of the BEM-FNO approach, we conducted simulation experiments on a set of 2D benchmark problems with various structures, including ellipses, Helmholtz resonators, and acoustic diffusers. We compared the performance of our approach with conventional BEM approaches and surrogate models based on convolutional neural networks. The results demonstrated that the proposed BEM-FNO approach can accurately and effectively solve the acoustic wave equation with varied structures and frequencies.

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Machine learning algorithms for accelerating material characterization, discovery, design, and manufacturing processes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LEARNING A RELIABLE COMPRESSION OF IN-SITU, HIGH-SPEED CAMERA DATA FOR ADDITIVE MANUFACTURING

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ABSTRACT

New experimental setups in additive manufacturing (AM) now allow for in-situ monitoring of the AM process via high-speed cameras centered at the point of interest. However, the volume of data generated from the high-speed camera even for a single layer of a build can be too large to store and analyze in a reasonable time frame. We propose utilizing a variant of autoencoders to learn a reliable compression algorithm from previous video data and show that the compressed representation encodes key quantities of interest relevant to the build quality, as well as the image reconstruction error. We discuss the limitations and benefits of our approach to in-situ monitoring of the AM process.

Multiphysics biomechanics of bio- and bio-inspired soft materials: Theory, simulation and experiments
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BACTERIAL MULTIPHYSICAL INTERACTIONS WITH HARD AND SOFT MATERIALS INTERFACES: TOWARDS COMPUTATIONAL DESIGN OF ENGINEERED LIVING MATERIALS

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ABSTRACT

Diverse sets of mechanisms underpin the ubiquity of bacterial interactions with surfaces and allow different bacterial species to adhere and proliferate. These mechanisms can often be effectively harnessed as guiding principles for producing materials for engineering purposes. For instance, microbially induced carbonate precipitation can help create new building materials that are less energy-intensive to manufacture and have lower lifetime operating costs. We computationally coupled multiphysical interactions in individual-based models to determine how bacteria form biofilm and biomineralize on patterned surfaces and in porous structures. Structural designs were proposed using data-driven modeling to optimize targeted biofilm properties, such as growth or adhesion. Similarly, differences in the molecular structures of healthy and diseased mucus in the human gut can alter the adhesion of bacteria on mucus. Intestinal mucus is the first line of microbial defense, a comparatively soft interface that allows for bacteria adhesion but obstructs penetration. We developed a coarse-grained mucus model that captured the molecular structures of two glycoproteins abundant in human gut mucus. Utilizing this model, we studied the dependence of nanoparticle diffusion on the particle size. Machine-learned fingerprints were employed to provide a mechanistic understanding of nanoparticle diffusional behavior. Our model provides a promising platform to study the pharmacokinetics in mucus.

Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A SIMPLE AND EFFICIENT FRAMEWORK FOR ADAPTIVE MULTISCALE MODELLING WITH DIRECT FE2

Kirk Ming Yeoh[*1], Karthikayen Raju[1], Leong Hien Poh[1], Tong-Earn Tay[1] and Vincent Tan[1]*

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ABSTRACT

While much more efficient compared to single scale models, computational homogenisation approaches remain unfeasible for large engineering structures. This is due to the sheer size of the model, as finely meshed representative volume elements (RVE) are included at every integration point of the macroscale mesh. In engineering structures however, the presence of various features as well as practical requirements result in only small regions of nonlinearity. As such, detailed RVE analyses are only required for such limited areas, while homogenised elastic properties can be used for the remaining areas of the macroscale structure.

As such, this work presents a simple and efficient framework to perform adaptive multiscale modelling with Direct FE2, where RVEs are progressively included into the analyses as necessary. Beginning with the unit strain analyses of the heterogeneous RVE, the framework first derives the homogenised macroscale elastic properties as well as the nonlinearity transition criterion for the structure. Subsequently, the main analysis is initiated with only the macroscale mesh and the homogenised properties.

As the analysis progresses, the macroscale integration point strains are checked against the nonlinearity transition criterion. If the criterion is satisfied, the macroscale element is first adapted into a Direct FE2 element before the analysis continues. For this adaptive process, the macroscale element is first assigned null properties. The deformed configuration of the RVE is then calculated before including it into the main analysis along with the scale transition relations. This check and adapt process is then repeated until the analysis is solved completely,

Compared to a full Direct FE2 model, such an adaptive approach can reduce the number of computations required significantly, by up to 50%. The proposed adaptive framework can be implemented entirely in Abaqus without the need to develop any subroutines. This means that the framework can be implemented by any user who is keen on multiscale modelling. More importantly, the entire process can be automated using Python scripts. Once the initial inputs are provided, no further user intervention is required, further simplifying the user task significantly. Several refinements are implemented to further optimise the adaptive framework and improve its efficiency.

MULTIPHYSICS PHASE-FIELD SIMULATION OF MICROSTRUCTURE EVOLUTION IN ADDITIVE MANUFACTURING

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ABSTRACT

Predicting the microstructure evolution during additive manufacturing (AM) is of great interests, which can complement the current time and cost expensive trial-and-error principle with an efficient computational design tool. However, it still remains a great challenge to simulate the microstructure evolution during AM due to the complex underlying physical phenomena. In this talk, I will present multiphysics simulations to capture the microstructure evolution during the selective laser sintering (SLS) and selective laser melting (SLM) AM process. The multiphysics simulations are based on our recently proposed thermodynamically consistent non-isothermal phase-field model including multiphysics (i.e. full or partial melting, pore structure evolution, diffusion, grain boundary migration, coupled heat transfer, grain coalescence, etc.), and interaction of powder bed and laser power absorption. The first part of the talk focus on the structural materials such as stainless steel. In the second part, we turn to the functional materials and take magnetic FeNi as an example to show our first attempt in simulating microstructure evolution and predicting magnetic properties by integrating finite element analysis, CALPHAD (CALculation of PHAse Diagrams), and micromagnetics.

Uncertainty quantification and reliability analysis in engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PROBABILISTIC FAILURE ENVELOPES OF MONOPILES IN SCOURED SEABED BASED ON A NEW NON-STATIONARY RANDOM FIELD MODEL

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ABSTRACT

Monopiles, which have been most extensively used in the offshore wind industries, are usually subject to threats from local scour. The effects of local scour on the bearing capacity of monopiles have been studied based on deterministic soil properties and local scour dimensions. However, both the properties of the seabed soil and the dimensions of the local scour have uncertainty. In this study, a new non-stationary random field model, which can better simulate the non-stationary characteristics of the seabed clayey soil and result in a safer probabilistic design of foundations, is proposed to characterize the spatial variability of the seabed clayey soil. Then, the effects of the spatial variability of the seabed clayey soil and the uncertainty of the local scour depth on the bearing capacity of monopiles are investigated under both uniaxial loading and VHM combined loading using random finite element method combined with Kriging meta-modeling technique and Monte Carlo simulation. The undrained shear strength of the seabed clayey soil was simulated with a log-normally distributed non-stationary random field and the local scour depth was treated as a uniform random variable. The negative correlation between them was also considered. The results show that the factor of safety required for the local scoured seabed decreases from 3.3 to 2.6 as the negative correlation enhances, greater than or equal to that (FS= 2.6) for the intact seabed. The procedure of analyzing the design failure envelop of monopile in spatially variable clayey soil with a local scour proposed in this study can provide a reference for geotechnical engineers.

Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICS-PRESERVING ENRICHED GALERKIN METHOD FOR THERMO-HYDRO-MECHANICAL PROCESSES IN GEOMECHANICS

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ABSTRACT

In this talk, we consider a new numerical method for thermo-hydro-mechanical (THM) processes described by Biot's thermo-poroelasticity model. Modeling THM systems has been a subject of great interest in various geomechanics applications, including thermal treatment for declogging wellbores, geothermal energy production, radioactive-waste disposal, etc. We will propose a coupled enriched Galerkin (EG) method utilizing two types of EG methods to provide a robust and physics-preserving method for the governing model. Specifically, the mechanics sub-problem is solved using a locking-free EG method, while the flow and heat sub-problems are solved using a locally-conservative EG method. The proposed method offers mass and energy conservation properties with much lower costs than other methods with the same properties, including discontinuous Galerkin methods and mixed finite element methods. Moreover, the new coupled EG method is free of common numerical instabilities that tend to appear in poroelasticity and coupled flow-transport simulations. We will discuss theoretical aspects of the new EG method, including mass and energy conservation properties and optimal convergence. We will also present some numerical examples to confirm the theoretical results and to demonstrate the robustness of the method in realistic scenarios.

FLUID COHOMOLOGY

Hang Yin[1], Mohammad Sina Nabizadeh[1], Baichuan Wu[1], Stephanie Wang[12] and Albert Chern[1]*

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ABSTRACT

The vorticity-streamfunction formulation for incompressible inviscid fluids is the basis for many fluid simulation methods in computer graphics, including vortex methods, streamfunction solvers, spectral methods, and Monte Carlo methods. We point out that current setups in the vorticity-streamfunction formulation are insufficient at simulating fluids on general non-simply-connected domains. This issue is critical in practice, as obstacles, periodic boundaries, and nonzero genus can all make the fluid domain multiply connected. These scenarios introduce nontrivial cohomology components to the flow in the form of harmonic fields. The dynamics of these harmonic fields have been previously overlooked. In this paper, we derive the missing equations of motion for the fluid cohomology components. We elucidate the physical laws associated with the new equations, and show their importance in reproducing physically correct behaviors of fluid flows on domains with general topology.

Model order reduction for parametrized continuum mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DYNAMIC MODE DECOMPOSITION OF NONEQUILIBRIUM GREEN'S FUNCTION FOR QUANTUM MANY-BODY SYSTEMS

Jia Yin[*1], Yang-hao Chan[2], Diana Qiu[3], Felipe Jornada[4], Steven G. Louie[5] and Chao Yang[1]*

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ABSTRACT

Simulating quantum many-body systems away from equilibrium is computationally challenging. To make it easier, a practical way is to examine the Green's function based on the many-body perturbation theory. However, the Kadanoff-Baym equations (KBEs) which describe the dynamics of the two-time non-equilibrium Green's function (NEGF) form a set of coupled nonlinear integro-differential equations difficult to solve. To deal with this problem, I applied DMD, which is a data-driven model order reduction technique, to simulate the long-time dynamics of the NEGF by using snapshots computed within a small time window. This technique was first applied to the time-diagonal of the two-time Green's function, and then to the off-diagonal elements by decomposing the Green's function into a number of one-time functions. The effectiveness of DMD is demonstrated on a two-band Hubbard model system. In the equilibrium limit, the DMD analysis yields results that are consistent with those produced from a linear response analysis. In the nonequilibrium case, the extrapolated dynamics produced by DMD is more accurate than a special Fourier extrapolation scheme. A potential pitfall of the standard DMD method comes from the insufficient spatial/momentum resolution of the discretization scheme. For the model system, this problem can be overcome by using a variant of DMD known as the higher order DMD (HODMD).

Computational fluid dynamics (CFD) and fluid-structure interaction (CFSI): Methods and Applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A SEQUENTIAL FLUID STRUCTURE INTERACTION ANALYSIS OF GAS SLAM CLOSURE OF FLAPPER SAFETY VALVES

Allan Zhong[1], Hadi Arabnejad[1], Terapat Apichartthabrut[1], Shengjun Yin[1], Shobeir Pirayeh Gar[1] and Junmei Zhang[1]*

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ABSTRACT

Downhole safety valves are a shut-in device that prevent the uncontrolled release of hydrocarbons in the event of a catastrophic incident from a well. These fail-safe valves typically incorporate a flapper type closure mechanism that is biased to close and is normally held open by an energized control mechanism. When the control mechanism is inactivated, the flapper gets caught into the flow and closes against the flow. This slam closure can cause damage to the hinge of the valve or to the flapper valve itself as the closing impact velocity is typically high due to the high fluid production rates. Because this valve is a safety device, it is important to ensure safe and effective operation of the valve post-closure. A safety valve system involves multiple components and a few control mechanisms. A fully coupled unsteady fluid-structure interaction (FSI) analysis is typically complex and requires intensive computational resources. A sequential Fluid Structure Interaction (FSI) methodology is developed to solve this challenge.

The first step of the sequential FSI analysis is the computational fluid dynamics (CFD) analysis. This step only considers the interaction between the flapper and the fluid where structural deformation is neglected. The CFD provides predictions of forces on the flapper valve as well as its angular velocity in addition to flow characteristics. The finite element model for structural dynamic analysis includes all components of the safety valve system and accounts for all interactions between the components. The control mechanisms in the system are modeled analytically and implemented through user subroutines to the FEA code. The effects of fluid on the structure are accounted for through CFD simulation and result in the force and pressure on the flapper valve as well as flapper's angular velocity. The force on the flapper predicted by CFD is applied in the FEA model and is monitored as a function of flapper angular position instead of time to improve the coupling between the CFD and FEA models.

The proposed sequential FSI methodology was calibrated by physical tests where the analysis predictions correlated well with experimentally observed results in terms of the location and extent of the potential damages. The sequential methodology proved to be very efficient computationally and has been successfully applied in regular design evaluations under different well conditions.

Design and mechanics of mutifunctional composites and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

INTEGRATED DESIGN AND PERFORMANCE ANALYSIS OF PEANUT PICKING MECHANISM

Yongran Yin[1], Yuguang Zhong[1], Dongyan Shi[1], Zeping Liu[1], Zhengyu Zhang[1] and Zeyi Wang[1]*

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ABSTRACT

Peanuts, as a vital oilseed crop, play a crucial role in global edible oil production and safety., and peanut picking is a highly complex nonlinear dynamics process. At present, the peanut picker has some problems, such as serious pod damage, low cleaning rate and straw blocking. Therefore, this paper proposes a movable integrated peanut picker for peanut picking and peanut straw crushing problems. Utilizing the structural characteristics of the separation drum and vibrating screen, the paper designed a peanut-picking mechanism to achieve a dual screening process for peanut fruits, and designed a crushing mechanism and incorporated dust-absorbing devices to ensure the efficient cleaning of crushed peanut seedlings, thus finalizing the integrated design of the peanut-picking machine. After the motion characteristic analysis and modal analysis, the rotating parts of the mechanism, the separation drum damage occurs mainly in the middle part, the rotating blade damage occurs in the tip of the top of the knife. And when operating the drum at 720 rpm, the primary blade at 1250 rpm, and the secondary blade at 950 rpm, this mobile peanut picker accomplishes the efficient screening of peanut fruits and the crushing of peanut seedlings. This study enhances both the efficiency and quality of peanut picking while providing a theoretical analysis and a foundational design basis for agricultural picking mechanisms.

Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL STUDY OF FRACTAL-TREE-GENERATED TURBULENCE

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ABSTRACT

We study the aerodynamics of fractal trees by using a simulation based on the Lattice Boltzmann Method with a cumulant collision term suitable for a large-eddy simulation model. We have applied L-SYSTEM[1] rules to construct self-similar fractal tree models in aerodynamic computations. We found that the drag coefficient closely matches that of real trees at high Reynolds number ($Re \geq 60{,}000$). A normalization process capable of collapsing turbulence intensity for various tree models is made. This process reveals that, at the same Reynolds number, different tree models exhibit the same behavior in the turbulence intensity of their wake region. On the other hand, in the case of the same tree model, when the Reynolds number is larger than 60,000, the turbulence intensity in the wake region exhibits the same behavior. Our assessment of global and local isotropy in the turbulence generated by fractal trees reveals that at high Reynolds number ($Re \geq 60{,}000$), the distant wake can be considered as nearly locally isotropic. Finally, the present numerical results confirm the non-equilibrium dissipation behavior previously observed in the case of space-filling fractal square grids[2]. In the wake region, the non-dimensional dissipation rate $C\epsilon \approx$ constant is not valid. Instead, it is inversely proportional to the local Taylor-microscale-based Reynolds number, $C\epsilon \propto 1/Re\lambda$.

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Advances in computational biomechanics and mechanobiology
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CONTINUUM-BASED PARTICLE MODELING FOR ELASTIC ANALYSIS OF MULTICELLULAR TISSUE MORPHOGENESIS

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ABSTRACT

Biological bone structures are determined through spatially heterogeneous cellular dynamics, such as hypertrophy and proliferation, which are affected by the mechanical and biochemical environment during morphogenesis. Therefore, to understand the mechanism of the formation of physiological bone structures, it is essential to investigate changes in the macroscopic tissue structure depending on microscopically heterogeneous cell activities. In this study, we aimed to connect microscopic cell activity to the elastic behaviors of the macroscopic tissue by developing a novel computational model of cell proliferation by extending the material point method (MPM), in which material points are used for the calculation of elastic deformation.

The growing bone tissue composed of chondrocytes and the surrounding chondrocyte matrix was modeled as a hyperelastic material following the compressible neo-Hookean model. We assumed that a material point in MPM represents a cell and surrounding matrix, to describe the individual cell activities during tissue morphogenesis. In this framework, we developed a continuum-based particle model of cell proliferation by combining unidirectional growth and division of material points [1].

Based on the developed model, we simulated random proliferation in multicellular cubic tissue. Macroscopic tissue growth and spatially heterogeneous cell volume and strain energy density were successfully simulated as a result of microscopic cell proliferation. Here, we confirmed that any cells in the tissue can be traced during tissue growth.

In this study, we developed a multiscale method to investigate multicellular tissue morphogenesis by constructing a continuum-based particle model of cell proliferation and enabled tracing cells in the growing tissue. Future extensions of the proposed models will allow us to consider cellular activities depending on the history of cell differentiation. Therefore, the developed model will contribute to understanding multiscale phenomena, such as cancer development and multicellular tissue morphogenesis forming various bone structures, through a computational approach.

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Machine learning for design tasks and inverse problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICS GUIDED TRAINING OF GAN MODEL TO IMPROVE ACCURACY IN A DESIGH SYNTHESIS

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ABSTRACT

In a mechanical design, a design that meets requirements has to be obtained. Deep generative models have been recently utilized for design synthesis. In literature, conditional generative models, such as conditional variational autoencoder (CVAE) and conditional generative adversarial networks (cGAN), are trained to generate designs with requirements as conditional labels. However, it is reported that the obtained shapes do not exhibit the same performance as the requirements. In this study, we use physics-guided GAN (PG-GAN) to improve accuracy in the design task for airfoils and ship hull shapes. In the GAN model, a discriminator distinguishes real data from fake data, but physics is not considered to distinguish reality, which leads to low accuracy in mechanical performance. In PG-GAN, reality is defined using a physics model; more precisely, if generated data is physically reasonable, the data are considered real, otherwise fake.

A physics informed neural network (PINN) is proposed in the literature to consider physics models. PI model uses the residual of the physics equations to be minimized. In PINN, he physics equations must be implemented in the neural network models to enable back propagation. Hence, general purpose software cannot be used. However, PG-GAN can use arbitrary physics models since the model is only used to label the generated data if the data is physically reasonable or not, and the physics model is outside the backpropagation chain.

The PG-GAN is applied to generate airfoil shapes and ship hull shapes, and the accuracy was improved.

REINFORCEMENT LEARNING-BASED TOPOLOGY OPTIMIZATION FOR ADAPTIVE METAMATERIAL USING WAVELET ACTION SPACE

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ABSTRACT

Ultrasound imaging is widely employed in medical and industrial fields due to its real-time capabilities, non-invasiveness, and cost-effectiveness. Despite these advantages, the inherent limitation of ultrasonic waves impeding their transmission through obstacles has spurred investigations into the utilization of metamaterials to overcome such hindrances. Notably, the variable characteristics of real obstacles, such as the human skull, across inter- and intra-subjects pose a significant challenge. Due to this variability, the efficacy of metamaterials designed for specific obstacles diminishes considerably in practical applications. The topology optimization methodology has been frequently used to identify optimal metamaterial designs meeting predefined design requirements. However, finding new optimal metamaterial designs in response to changes in the circumstances surrounding the design domain remains a challenge.

This research introduces a novel topology optimal design methodology aimed at robustly and efficiently creating adaptive metamaterials by harnessing the real-time response capabilities of reinforcement learning. In addressing a limitation of existing reinforcement learning-based methodologies, namely the exponential increase in training time with resolution, we propose the innovative concept of a “wavelet action space.” To overcome the issue posed by resolution-dependent training time, we converted the space where the reinforcement learning agent selects actions into a multi-scale action space using binary wavelet transformation. This approach enabled multi-resolution design by constraining the range of actions that the agent could choose at each design step. The outcome of this research includes the successful training of an agent capable of altering metamaterial geometry to facilitate the penetration of ultrasonic waves through obstacles with varying thicknesses, achieving an efficiency exceeding 90 %. This pioneering methodology is expected to establish a significant milestone in the emerging reinforcement learning-based topology optimization design field, offering promising avenues for further exploration and advancement.

Advance modeling and simulation in complex porous media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PORE-SCALE REACTIVE TRANSPORT AND FLOW BEHAVIOR INVOLVING DISSOLUTION AND PRECIPITATION IN HETEROGENEOUS POROUS MEDIA

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ABSTRACT

Recent advances in experimental methods and multi-scale imaging capabilities have revolutionized our ability to quantitatively characterize flow and transport processes in porous media. Reactive transport and chemical reactions involving phase change take place in pores and along the mineral surfaces in confined porous media. These coupled reactive transport processes are critical to various subsurface applications such as subsurface resource recovery, carbon sequestration, and environmental fate and transport. In this work, pore-scale experiments in single fractured systems including calcite and cements are used as a basis for understanding coupled processes among hydrodynamics, transport, and reactions at the (sub) pore-scale. Optical and confocal microscopic imaging at multiple scales from ~0.1 to 5 micron resolutions will be used to trace how these chemical reactions will induce the change of morphology on single fracture surfaces via dissolution and precipitation. These experimental data will be analyzed by developing coupled pore-sale simulation using the hybrid lattice Boltzmann method for flow and finite volume method for reactive transport. Once pore scale simulations are validated against well-controlled experimental data, we utilize pore scale simulations to generate a number of datasets under a range of key parameters including the Peclet and Damkhöler numbers with different geometries. Dissolution and precipitation dynamics especially affect the flow field, resulting in transient behavior of reactions. We will show how these data can be utilized to train a machine learning model for upscaled reactive transport parameters. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

Isogeometric methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SHAPE DESIGN OPTIMIZATION OF MAGNETIC ACTUATOR USING ISOGEOMETRIC BOUNDARY ELEMENT METHOD

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ABSTRACT

A continuum-based shape design sensitivity analysis (DSA) method is developed for two-dimensional multi-domain magneto-static problems using the isogeometric boundary element method (IBEM) that directly utilizes NURBS basis functions in CAD systems in response analysis. Since the compatibility condition between the NURBS patches for multi-domain problems in BEM should be satisfied, discontinuous element formulation is adopted. Especially for a surrounded domain for all directions in an inhomogenous multi-domain problem such as magnetostatics, additional imposition of material property is introduced. Generally, the magnetic potential has a strong dependency on the geometry of ferromagnetic materials, and the exact boundaries of multi-domain are expressed using the NURBS basis function and control points in response analysis. Consequently, the developed isogeometric shape DSA method gives more accurate information as the gradient of the objective function for guiding one directional search in optimization. Through the numerical examples, the robustness of developed discontinuous IBEM and DSA is demonstrated.

Minisymposium in honor of Prof. Yannis Kallinderis's 60th birthday: Progress of Unstructured grid based CFD, hybrid mesh generation and adaptation, and parallel supercomputing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL SIMULATIONS OF BREAKING WAVES

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ABSTRACT

We present numerical simulations of free surface flow problems[1], specifically focusing on breaking wave phenomena that include spilling and plunging breaker. The incompressible Navier-Stokes equations are solved using the weighted essentially non-oscillatory (WENO) scheme, ensuring accuracy[2]. For capturing the moving immiscible interface, the tangent of hyperbola for interface capturing with weighted line interface calculation (THINC/WLIC) method is employed. Wave breaking processes are presented and discussed through interface diagrams and energy dissipation. The result of the present simulation compares well with other numerical results and is successfully applied to breaking wave phenomena.

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Imaging and computational methods for biomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CONTROLLING ENZYME ORIENTATION FOR OPTIMAL ELECTRON TRANSFER ON BIOELECTRODE SURFACES THROUGH ELECTRIC FIELD MODULATION: INSIGHTS FROM MOLECULAR DYNAMICS INVESTIGATION.

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ABSTRACT

Developing bioelectrochemical devices requires the critical surface immobilization of biocatalysts with a favorable orientation. Enhancing the performance of electrochemical electrodes has traditionally involved complex and costly processes for biocatalyst surface modification and engineering. One proposed method for achieving proper biomolecule orientation and deposition on the surface involves applying an external electric field (EF) to small molecules. In this study, we introduced a unidirectional external EF for the first time to oxygen-reducing enzymes with high catalytic activity. Using computational methods, we constructed a Laccase-graphene interface. The applied external EF induced rotation of the active site of laccase, leading to an improved electron transfer rate compared to enzymes physically immobilized on graphene. We also evaluated the external EF fabrication process for different graphene congeners (graphene oxide (GO) and reduced GO (rGO)). The electrode surface morphology was visualized, and computational methods were employed to confirm binding conformation, dipole moment orientations, secondary structure, and binding stability. Among the graphene materials tested, graphene exhibited the most promise, surpassing GO and rGO by 10% and 5%, respectively, in terms of DET rate. These findings suggest that employing an external EF to achieve a favorable orientation in the Laccase-graphene interface could represent a straightforward, cost-effective, and efficient approach for bioelectrode fabrication.

Advanced multi-physics CFD simulations in science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMPACT OF SURFACE ROUGHNESS ON TURBULENT TRANSITION ON A HIGH REYNOLDS NUMBER INFINITE SWEPT WING

Hayahide Yoshida[*1], Takahiro Ishida[2], Keisuke Ohira[3], Ryo Araki[1] and Takahiro Tsukahara[1]*

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ABSTRACT

The boundary layer near the leading edge of a conventional swept-wing aircraft is dominated by instability of the crossflow perpendicular to the streamline direction. This instability arises as a disturbance originating from surface roughness and promotes the turbulence transition. There are wide variety of shapes in the aircraft wing surface roughness, and the complex interference of disturbances from various roughness leads to the turbulent transition. In particular, at high Reynolds numbers of order O(10^7) corresponding to actual flight conditions, the boundary layer is so thin that even very slight roughness influences the transition. However, both flight tests and wind tunnel experiments of the surface roughness-induced transition in the actual flight conditions are demanding and costly.

In this study, we aim to elucidate the relationship between the surface roughness and the transition position of an infinite swept wing (TAMU0706 [1]) under Reynolds number equivalent to the actual flight. We employ Reynolds-averaged Navier-Stokes (RANS) equations including laminar flow region for the external flow surrounding the entire wing. For the vicinity of the wing surface with roughness, we employ direct numerical simulation (DNS) where the boundary condition for the outer flow is given by the RANS simulation. The turbulent transition position located far downstream is determined using the nonlinear parabolized stability equations with the disturbance amplitude obtained by the DNS. With this combined method, we can investigate the roughness-induced flow accurately while maintaining low computational cost .

Our analysis unveiled the relationship between the turbulent transition position and the roughness properties, such as the arithmetic mean roughness (Ra) and spatial distribution. The transition position advances to leading edge by increasing Ra, and above the critical Ra, the turbulent transition occurs immediately from the leading edge. Even for the same Ra, the spatial distribution of roughness influences the transition position. In addition, we found a range of the roughness wavelength that does not affect the transition position. In the presentation, we will discuss some other roughness shape parameters, such as the maximum roughness height and the root-mean-squre value of the roughness.

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PHASE-FIELD MODEL FOR VISCOUS DOMINATED HYDRAULIC FRACTURING

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ABSTRACT

With increasing popularity in versatile fracture problems, phase-field models have been applied for hydraulic fracturing by extending the Francfort-Marigo energy functional to poroelastic media. However, when hydraulic fractures propagate in a viscous-dominated regime, in which the surface energy dissipation is negligible compared to the fluid viscous dissipation, existing phase-field models become unstable and often lead to non-localized phase-field (damage) profiles. In this presentation, we propose a micro-poroelastic based phase field fracture model to overcome the non-localized damage and pore-pressure profiles. The proposed model allows for a variationally consistent formulation and rational derivation of effective stress and phase-field--dependent poroelasticity. The fixed stress split scheme was applied to solve the hydro-mechanical coupling problem which includes two independent pressure variables. We first verified this model against typical micro-porosity problems and then extended it to viscous-dominated hydraulic fracture examples.

Biomechanics of hard tissues: From experiments and simulations to clinical applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AUTONOMOUS FINITE ELEMENTS COMBINED WITH DEEP LEARNING IN ORTHOPEDIC AND ENDOCRINOLOGY CLINICAL PRACTICE

Zohar Yosibash[1], Nir Trabelsi*[2] and Amir Sternheim[3]

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ABSTRACT

Finite element analysis requires a qualified analyst to generate the necessary input data, verify the output and post process the analysis results for a meaningful conclusion. The required expertise and labor efforts precluded the use of FEA in daily medical practice for example. Recent scientific advancements such as low dose CT scans, machine learning, and high order FEA which allows an inherent verification methodology of the numerical accuracy, make it possible to provide a fully autonomous process for assessing bone strength and fracture risk.

This autonomous process, named autonomous finite element (AFE) analysis, introduces a paradigm shift in the use of FEA. This talk addresses a novel AFE for patient-specific analysis of human femurs used nowadays in clinical practice: it involves an automatic segmentation of femurs from CT-scans by U-Net, an automatic mesh generation and application of boundary conditions based on anatomical points, a high-order FE analysis with numerical error control, and finally an automatic report with a clear assessment of bone fracture risk. Two specific applications of AFE in clinical practice that were validated by clinical trials are presented:
a) Determination of the risk of fracture for patients with tumors of the femur and whether a prophylactic surgery is needed.
b) Identifying patients with high hip fracture risk as a result of fall on the side.

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DEEP GENERATIVE APPROACH FOR BIOINSPRIED STRUCTURAL MATERIALS BY DESIGN

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ABSTRACT

The fusion of Artificial Intelligence (AI) with bioinspired structural materials design represents a groundbreaking shift in material science, merging the complexity of nature's designs with the precision of modern engineering. By harnessing deep learning and reinforcement learning, AI accelerates the development of materials that mimic natural structures, offering efficiency and resilience unmatched by traditional materials. This integration significantly shortens the pathway from conceptual design to practical application, with AI's ability to analyze large datasets from simulations and empirical studies playing a key role. It enables a deeper understanding of the behaviors of natural materials, paving the way for the engineering of novel structures that aim to exceed the performance of their biological inspirations.

Moreover, AI enhances the manufacturing processes of these bioinspired materials, optimizing production to ensure quality while prioritizing sustainability. This optimization aligns with the global push towards reducing waste and energy consumption, heralding a new era of materials with unparalleled properties and environmental benefits. The collaboration between AI experts and material scientists accelerates innovation, leading to sustainable material development and the creation of cutting-edge materials. As AI technologies continue to evolve and become more integrated with bioinspired design, the potential for creating materials with superior performance characteristics expands, promising a future where the synergy between nature's ingenuity and AI's analytical prowess sets new benchmarks in material innovation and sustainability.

Complex fluid flows in engineering: Modeling, simulation, and optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTATIONAL ANALYSIS OF THE FINITE IMMERSION DEPTH DIP COATING PROCESS

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ABSTRACT

Dip coating with finite immersion depth is a newly defined coating process which has both characteristics of the conventional dip coating and the liquid transfer process. In contrast to its wide range of industrial applications, studies on the dip coating with finite immersion depth are limited due to the complexity of analysis. Since most conventional dip coating studies assume a very long immersion depth of the substrate, the coating layer thickness which is a function of the dimensionless numbers becomes uniform above the dynamic meniscus region and thus the steady-state studies can be performed. However, due to the relatively short immersion depth compared to conventional dip coating, the finite depth dip coating does not guarantee an uniformity of the film thickness. Furthermore, due to the severe topological changes in the liquid, which is one of the characteristics of the liquid transfer process, studies should be performed in a transient way. Unlike the liquid transfer process, which moves the liquid from the cell or groove to the substrate, the liquid source has no contact lines in the dip coating with finite immersion depth. In addition, there is an effect of viscous drag originated from the vertical wall which is one of the characteristics of the conventional dip coating process.

In this study, we implement the computational model to understand the dynamics of the liquid and the interface in the finite immersion depth dip coating by combining the interface treatment schemes. We utilized the phase field method, which is one of the well-known interface capturing schemes, to describe the movement of the liquid-air interface. On the other hand, we moved the nodal points with the scheme of Arbitrary Eulerian Lagrangian(ALE) method for the movement of the solid substrate. To analyze the process, we divided the process with several stages based on the onset of its characteristics. Then we track the change of the quantities of the spatial regions divided by the specific horizontal planes with respect to the characteristics of each stage. Comparing the changes of the quantities between different parameters, we find out how much the process parameters affect the formation of the coating layer shape. In addition, the simple model which describes the major dynamics will be presented.

Machine learning algorithms for accelerating material characterization, discovery, design, and manufacturing processes
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A DATA-DRIVEN METHOD FOR MECHANICAL PROPERTIES PREDICTION OF MATERIAL BUILT BY METAL ADDITIVE MANUFACTURING

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ABSTRACT

Metal additive manufacturing (AM) represents a transformative and advanced technology characterized by low cost, short production cycles, and integrated design and manufacturing processes. It holds vast potential and promising prospects in aerospace, nuclear power, and medical applications. However, the as-built material by AM presents a complex microstructure and inevitably contains manufacturing defects. Therefore, developing accurate and efficient methods for mechanical property prediction is crucial for predicting the actual performance of manufactured parts. In this study, a crystal plasticity finite cell - self-consistent clustering analysis method (CPFC-SCAM) is presented. It consists of an offline data preparation stage and an online rapid calculation stage. During the offline stage, the crystal plasticity finite cell method and clustering algorithms are applied to construct a discrete database of the actual microstructure representative volume elements (RVEs) efficiently. In the online stage, the Lippmann-Schwinger equation of the RVEs is solved by the subdomain-based weighted residual method with the clusters from the offline stage. The crystal plasticity model under finite deformation is utilized in the CPFC-SCAM. The macroscopic equivalent mechanical properties of the material are obtained through the homogenization of stresses and strains within the RVE. Several numerical examples, RVEs with and without the irregular void, are presented to showcase the accuracy and efficiency of the proposed method. Moreover, the proposed method is applied to study the mechanical properties of IN625 alloy fabricated by selective laser melting AM. The results demonstrate that this work provides an efficient computational method for predicting the mechanical properties of the built material by metal AM.

Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SPATIAL AND TEMPORAL CONSTRAINTS OF THE COHESIVE MODELING: A UNIFIED CRITERION FOR FLUID-DRIVEN FRACTURE

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ABSTRACT

We present a unified criterion for cohesive modeling of fluid-driven fracture based on the dimensional analysis to simultaneously provide the constraint for cohesive element and time step sizes. Complicated by the nonlinear interaction between solid deformation and fluid flow, the underlying correlation between discretization and physical parameters of fluid-driven fracture is still unclear. This work studies this correlation through the dimensionless process of the governing equations that associate the cohesive element and time step sizes in a discrete regime. Three characteristic parameters (i.e., related to crack opening, fluid pressure, and fracture length) are introduced in the derivation, and two dimensionless parameters are proposed to construct the unified criterion. The criterion is validated by numerical tests of toughness-dominated fracture with various conditions including the modulus of solid, injection rate of fluid, fracture energy, and in-situ stress. The proposed criterion determines the spatial and temporal constraints of the cohesive zone model (CZM) for modeling fluid-driven fracture, which is often treated empirically in previous practices.

The phase field method for fracture: Theory, numerics, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFECT OF THE RATIO OF DIFFUSE LENGTH SCALE AND IRWIN'S MATERIAL CHARACTERISTIC LENGTH SCALE L0/LCH ON THE PHASE FIELD MODELING TO BRITTLE OR QUASI-BRITTLE FRACTURE

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ABSTRACT

In the phase field model (PFM), the discrete crack is diffused, which enables to deal with complex fracture patterns for brittle or quasi-brittle materials. The classical PFMs lack of the information on the material strength. To capture the material strength, the length scale l0 of the diffuse crack is tie to the characteristic length lch of the crack process zone. The ratio of l0/lch usually remains constant for the classical PFMs, resulting in the size scale of the diffuse crack is limited by the material properties. To overcome this limitation, we construct novel degradation functions to decouple the diffuse length scale l0 from the characteristic length lch, making the ratio of l0/lch adjustable whether to small or to large. Based on the analysis of the homogeneous solutions for 1D tension under various diffuse crack topologies, the effect of the ratio of l0/lch on the constitutive behaviors of the PFMs is investigated. It is found that the appearances of the elastic phase and the strain hardening phase as well as the softening law are influenced by l0/lch. For a large value of l0/lch, the snap-back instability occurs and the constitutive behavior showcases very brittle. For a small value of l0/lch, the constitutive behavior is very ductile with no elastic phase. When the ratio of l0/lch increases, the fracture type is transformed form quasi-brittle to catastrophe. As a consequence, the ratio of l0/lch, a nondimensional number, governs the competition between the strain energy and surface energy in the PFMs.

Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THERMO-HYDRO-MECHANICAL COUPLED MATERIAL POINT METHOD FOR SIMULATING THE FREEZE-THAW BEHAVIOR OF POROUS MEDIA

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ABSTRACT

Climate warming is causing disruptions in the normal freeze-thaw cycles of permafrost and seasonal frost regions. This leads to an increase in climate-driven disasters such as ground collapse and retrogressive thaw slumps, which pose increased risks to the stability of infrastructure in cold regions. However, understanding and predicting the freeze-thaw behavior of ice-rich porous media is challenging due to its inherent complexities. These include multiphysics and multiphase interactions, phase transitions, ice-dependent constitutive behaviors, fluid-like failure patterns, and large deformations. To address these challenges, this study presents a thermo-hydro-mechanical coupled MPM framework for modeling time-dependent phase transition and large deformation behaviors. The framework includes four features: (a) fully coupled u-v-p-T governing equations to describe the interactions of heat transfer, pore-liquid flow, and solid deformation in freezing and thawing porous media based on single-point multiphase MPM, (b) a soil freezing characteristic curve and relative hydraulic conductivity model to describe the phase equilibrium and the influence of ice saturation on permeability, (c) an ice-saturation dependent Mohr-Coulomb model to characterize the effect of ice cementation on soil strength, and (d) a fractional-step-based semi-implicit integration algorithm to solve the coupled formulations.

The presented framework is validated by several thermo-hydro-mechanical coupled examples to demonstrate its effectiveness in simulating thermal variations due to heat conduction, convection, and latent heat of fusion, mechanical behaviors due to thermal expansion/contraction and liquid-ice phase transition, and hydraulic changes due to ice saturation and porosity variations. The semi-implicit MPM formulation is shown to maintain both satisfactory numerical stability and computational efficiency when dealing with nearly incompressible fluids and extremely low permeability conditions in frozen porous media. Finally, the framework is used to simulate a thawing-induced slope slide and the large settlement of a strip footing placed on a thawing ground. The results showcase the significant influence of strength reduction during ice melting on the stability, bearing capacity, and failure pattern of ice-rich soils. This study presents a powerful tool for predicting the impact of climate warming on engineering practices in cold regions. It can be further enriched by employing a multiscale approach (e.g., MPM-DEM) and a fracture model to model more comprehensive behaviors in ice-rich soils.

Acknowledgments: The study was financially supported by RGC/GRF 16211221 and CRF C7082-22G.

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Battery modeling and computation: From material to device
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A COMPARATIVE STUDY OF THE STATE OF CHARGE ESTIMATION FOR LITHIUM-ION BATTERIES USING SINGLE PARTICLE MODEL AND KALMAN FILTER

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ABSTRACT

Effective and accurate state of charge estimation for lithium-ion batteries is of paramount importance for reliable and safe operations of lithium-ion batteries and it is an important function of the battery management system. At present, a popular applied scheme involves coupling an equivalent circuit model (ECM) together with a Kalman filter. ECM employs electric circuit elements, like resisters and capacitors, to mimic the cell voltage response given an input current load. The model relies on experimental data for calibration; hence inherently, it is limited for model extrapolation and predict less accurately in the loading situation where the experimental data does not cover well. Therefore, in literature, there is growing interest in using a single particle model (SPM) with a Kalman filter for state of charge estimation. SPM is a simplified physics-based model, considering each electrode as a single spherical particle whose area represents the porous electrode active surface area. SPM accounts for solid diffusion in the electrode particles and the intercalation reaction kinetics. The ohmic potential drop in the electrolyte is incorporated using a lumped solution resistance term. To couple with the Kalman filter, it is necessary to convert SPM into the state-space formulation. In literature, there is little consensus on how such conversion should proceed. Among the many proposed approaches, two more different schemes are mentioned: (1) discretizing both solid diffusion equations directly using finite difference and (2) solving the diffusion for the internal states of “only one” electrode and recovering the states of the other electrode using algebraic expression to “enhance model observability”.
Here, we present a comparative study on these two coupling schemes of SPM with two popular nonlinear Kalman filters. We evaluate their accuracy and required resolution time, as well as investigate the importance of enhancing the model observability. The results provide useful insights on how to address the implementation challenges faced in real-life applications.

Predictive digital twins
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPUTER MODELLING OF FLASH SINTERING

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ABSTRACT

Flash sintering is a time-efficient and energy-saving method compared to traditional sintering. However, due to the high heating rate and the nature of ceramic sintering, deformation and distortion can occur during the process. This is where computer modelling becomes instrumental. It allows us to analyse and predict the conditions of deformation and distortion during the flash sintering process. By understanding these behaviours, we can pre-adjust the green body (pre-sintered ceramic) and sintering conditions to achieve an optimal outcome, leading to a substantial reduction in material waste and energy cost. Therefore, this study aims to predict the heating and deformation conditions of a ceramic part undergoing the flash sintering process.

In this study, we will simulate the flash sintering process of a ceramic part using COMSOL Multiphysics. We will apply a pair of cathode and anode to the green body using Electric Potential functions. Due to the Joule heating effect, these will cause localised high temperatures in the ceramic part, leading to regionally increased sintering and creeping rates. This can result in a non-uniform distribution of temperature in the ceramic part, preventing it from being evenly sintered and causing non-uniform deformation. This becomes critical when the sintered part is dimensionally sensitive. We will carry out a series of simulations to simulate the Joule heating effect during the flash sintering process, yielding the distributions of electric potential and temperature in the ceramic part. We will also simulate its sintering behaviour, yielding the temporal evolutions of grain size and relative density.

This study establishes a foundational procedure for predicting ceramic flash sintering deformation through finite element analysis methods. It demonstrates the effectiveness of this approach for deformation prediction in the ceramic flash sintering process, potentially leading to a reduction in material waste and energy costs. The simulation outcomes validate this approach for predicting flash sintering deformation, providing a basis for further research in this field.

Fracture, damage and failure mechanics of cementitious materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL MODELLING OF THE DYNAMIC FAILURE IN FIBER-REINFORCED CONCRETE

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ABSTRACT

We present a two-level model for cement-based composites reinforced with fibers.

First, the pull-out behavior of a single fiber from the matrix is modeled and validated against experimental results. At this mesoscopic level, the fiber can be smooth or with hooked ends, based on the explicit representation of the fiber, the cementitious matrix and the interface in between. Consequently, the effect of friction, loading-rate dependency, in particular, the fiber orientation, are cast into an equivalent constitutive law for each fiber at a given orientation. Numerous simulations are performed to create a database of fiber behavior with different orientations.

Second, at the macroscopic level, the fibers are fed with constitutive relations from the previously generated database. A notched three-point bending beam with a central cohesive crack sewed with fibers is modeled and the global response validated against experimental results.

Third, the same concept is applied to a mixed-mode fracture propagation. A fiber distribution is generated based on images obtained from micro Computerized Tomography scanning. In this case, the constitutive relation for each fiber is activated according to the current principal stress directions. The global response is also compared with its experimental counterpart.

Lattice Boltzmann modelling and study of complex flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LATTICE BOLTZMANN METHOD FOR FLOWS AND TRANSPORT IN POROUS MEDIA BASED ON ADAPTIVE MESH REFINEMENT

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ABSTRACT

In accordance with the weakly compressible flow model proposed by Qian [1], and the incompressible flow model introduced by Guo [2], a numerical simulation solver for the flow and transport in porous media with lattice Boltzmann method (LBM) under the AMROC(Adaptive Mesh Refinement in Obiect-oriented C++) [3] framework was established via the massively parallel adaptive mesh refinement (AMR). The flow characteristics in porous media was carried out by employing the established AMR-LBM model. The effects of different pore structures (ordered and disordered structures), porosity, Reynolds number(Re), and inlet conditions on the flow evolution were investigated in detail. The flow process associated with velocity, velocity vector, and vorticity under various physical property parameters was obtained. The numerically obtained results of varying structures and flow conditions were analyzed so as to gain a good performance of flow ability and transport capacity. The current investigation combines the advantages of LBM in dealing with pore structure easily and AMR technology, which ensure numerical accuracy and also improve computing efficiency owing to the high refinement strategy of AMR technique. The obtained results were also verified by the previous experimental results, which proves the accuracy and robustness of the current numerical simulation. It is hoped that this study could extend the numerical simulation ability in the massive parallel simulation and AMR technology in the LBM community.

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DESIGN OF HIERARCHICAL MICROSTRUCTURES WITH ISOTROPIC ELASTIC STIFFNESS

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ABSTRACT

Microstructured metamaterials are a class of artificial materials with rich geometric configurations. By designing their geometries, they can achieve extraordinary properties that cannot be found in natural materials, such as negative Poisson's ratio, bimodal properties, etc[1]. In recent years, rapid advance of 3D printing technology offers a unique way to fabricate high-resolution microstructured metamaterials with various configurations[2]. Among various properties, elastic stiffness is one of the most fundamental properties. Particularly, the microstructures with isotropic stiffness are insensitive to changes of loading directions and suitable for complex conditions, and thus they have attracted great interest from researchers[3]. To date, most isotropic microstructures are designed either based on mechanics principles or by using numerical optimization strategies. However, because of the limitation of the design space and modelling methods, the existing isotropic microstructures are composed of features in a single length level. Exploring a wider range of isotropic microstructures becomes a key and also an open problem.

This paper identifies a new family of isotropic microstructures by introducing hierarchical features, which is called the Isotropic Hierarchical Microstructures (Iso-HMs). They are made by introducing another level of features into the solid parts of the original single-level microstructures, which have orthotropic stiffness. By designing the second-level microstructures and adjusting the geometric parameters, isotropic stiffness can be realized. Numerical results show that both the Young’s modulus and shear modulus of the Iso-HMs are bigger than the minimal directional stiffness of the single-level microstructures. Furthermore, Iso-HMs can achieve over 50% improvement of the buckling strength compared to the single-level counterparts, when subjected to a uniaxial loading. Several specimens were 3D printed by using the Projection Micro-Stereolithography technology. The minimal feature size was 50 micro-meter, and the size ratio between the specimens and the minimal features reached 400:1. The testing results from the uniaxial compression also demonstrate the stiffness isotropy of the specimens. Such a hierarchical design significantly expands the already-known space of isotropic microstructures.

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The phase field method for fracture: Theory, numerics, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN ADAPTIVE INCREMENTAL STAGGERED SCHEME FOR THE PHASE FIELD MODEL OF FRACTURE

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ABSTRACT

For the standard staggered solution scheme widely used in phase field model, although it shows excellent convergence and robustness, the computational efficiency is slow and a large number of iterative steps are required, resulting in huge time cost. In order to improve computational efficiency, an efficient and robust solution scheme based on adaptive time field is proposed. This scheme is inspired by the space field adaptive mesh method, and an error indicator based on phase field and history field variables is established. The time field is coupled with the phase field and energy field in the space field, allowing the time step to adaptively adjust with iteration, improving convergence rate and significantly reducing time cost. The proposed scheme is validated through some representative examples. The results indicate that the presented scheme not only significantly improves computational efficiency, but also has accurate computational results. Compared to the standard staggered scheme, the time cost of the presented scheme is less than 4% of the time of the standard scheme. Furthermore, this novel scheme can effectively reduce the impact of load increment in the standard scheme on the results, improve stress distribution, and enable cracks to propagate along the correct path. What's more, the presented scheme has a faster computational efficiency than the monolithic BFGS scheme and excellent convergence characteristics.

Keywords: staggered scheme; phase field method; error indicator; adaptive time field; monolithic scheme

TOWARD FOUNDATION MATERIAL MODEL WITH NONLOCAL ATTENTION OPERATOR

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ABSTRACT

Despite the recent popularity of attention-based neural architectures in core AI fields like natural language processing and computer vision, their potential in modeling complex physical systems has been relatively underexplored. Unlike traditional machine learning tasks, physical systems in real-world applications feature scarce measurements and changing hidden states, and therefore calls for an automated self-adaptive mechanism capable of evolving continuously with the current state of system. To this end, we consider the learning of material responses as an exemplar complex physical system modeling problem, and investigate the self-adaptive capability of attention mechanisms toward developing a foundation material model. Specifically, we first show that the attention mechanism is equivalent to a nonlocal neural operator with data-dependent kernels, such that enables the automatic updating of the evolving physical properties via the attention matrix. We then propose Nonlocal Attention Operator (NAO), which provides a forward model in the form of nonlocal constitutive law, ensuring adherence to fundamental physical laws. In a wide variety of scientific applications ranging from constitutive modeling of material deformation, stress wave propagation, to digital twin modeling, we empirically demonstrate the advantages of NAO over the baseline neural operators and state-of-the-art methods in capturing the change of hidden physical states.

Imaging-based methods in computational medicine
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEEP LEARNING ENHANCED POLYCUBE METHOD FOR HIGH-QUALITY HEXAHEDRAL MESH GENERATION AND VOLUMETRIC SPLINE CONSTRUCTION

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ABSTRACT

In this study, we present a novel algorithm that integrates deep learning with the polycube method to generate high-quality hexahedral meshes, which are then utilized to construct volumetric splines for isogeometric analysis. Our algorithm begins by establishing a connection between surface triangular meshes and polycube structures. We employ deep neural network to effectively classify and transform surface triangular meshes into their corresponding polycube structures, thus capturing relevant spatial structural information of the geometry models. Following this, we combine the acquired polycube structural information with unsupervised learning to execute precise segmentation of surface triangular meshes. This step overcomes the sensitivity to the initialization and the noise encountered in traditional polycube methods, but also significantly enhancing the segmentation results while reducing the requirement for manual intervention. Quality hexahedral meshes are then generated from the polycube structures, employing octree subdivision and mapping techniques. The incorporation of deep learning for creating polycube structures, combined with unsupervised learning for segmentation of surface triangular meshes, substantially elevates the efficiency and quality of mesh generation. Finally, truncated hierarchical B-splines are constructed on the generated hexahedral meshes. We extract trivariate Bézier elements from these splines and apply them directly in isogeometric analysis. This study also offers several examples to demonstrate the robustness of our algorithm.

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Boundary element methods: New theories and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

UNIVERSAL CONTACT STIFFNESS OF AXISYMMETRIC INDENTATIONS CONSIDERING THE EFFECT OF MEMBRANE TENSION ON THE SURFACE

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ABSTRACT

Many biological systems exhibit in-plane membrane tension on their surfaces, a factor often overlooked in existing indentation analyses despite its significant impact on contact responses. This presentation introduces a boundary element method designed to address the normal contact problem of elastic solids covered with thin tensed membranes. Utilizing this method, we calculate the contact stiffnesses associated with indentations using various axisymmetric indenters. Notably, the membrane tension effect leads to contact stiffness values considerably higher than those predicted by conventional theories (e.g., Hertz theory, Sneddon's solution) when the contact size diminishes to the same order as the ratio of membrane tension to elastic modulus. Theoretically, we found that the contact stiffness of arbitrary convex indentations can be universally expressed as a function of contact radius, with an explicit expression derived by modifying conventional solutions. Building on this universal contact stiffness, a straightforward analysis method is proposed to estimate the membrane tension and elastic modulus of biological systems using experimentally recorded indentation load-depth data. This approach proves useful in analyzing indentation experiments conducted on cells and lungs.

Current trends in phase-field modeling and computations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHASE FIELD METHOD BASED ON REDUCED-ORDER-HOMOGENIZATION FOR FIBROUS COMPOSITE MATERIAL

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ABSTRACT

This report proposes a novel multiscale phase field method (PFM) based on reduced-order-homogenization (ROH) approach to investigate the damage evolution for the fibrous composite material, namely the ROH-PFM. In the ROH-PFM, the matrix phase is described by the PFM, and the fiber phase could be modeled by some other classic constitutive model. The overall response of the fibrous composite material then is obtained by averaging and homogenization approaches through the ROH framework in order to obtain the macro-scopic stress and consistent material moduli. In the present work, we derive the governing equations in terms of the displacement field and the matrix phase field. Through the ROH and the Francfort–Marigo variational principle, we can obtain the governing elliptical partial differential equation for the matrix phase field in terms of the stress states of the matrix and fiber phases. The corresponding weak form is derived, and numerical algorithm through the finite element method is derived as well. Finally, three groups of numerical simulations are selected to verify the functionality of the ROH-PFM, while the fibers are assumed to follow an isotropic continuum damage model. The numerical examples show good performance of the ROH-PFM in stating various material degradation mechanism.

Modeling and inverse design of architected materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEEP LEARNING FOR MICROSTRUCTURE DESIGN OF VISCOELASTIC COMPOSITES WITH DESIRED RELAXATION MODULI

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ABSTRACT

Viscoelastic materials are widely used in various engineering applications including vibration damping, acoustics, tissue engineering and medical devices. Despite the versatility of viscoelastic materials, it is hard to find one that exhibits the desired relaxation moduli. Composite materials can produce the desired relaxation moduli by designing microstructure.

In this research, a design methodology based on deep learning is developed to find the microstructure of viscoelastic composites with desired relaxation moduli. The viscoelastic composites are assumed to be composed of periodic unit cells. Various shapes of unit cells are generated as initial data sets by performing topology optimization for either maximizing the bulk modulus, the shear modulus or minimizing the Poisson's ratio. Variational autoencoder (VAE) and generative adversarial network (GAN) are trained by using the initial data set and they generate more diverse microstructures. The relaxation modulus of each microstructure is calculated through the numerical homogenization method. Since the relaxation moduli are time-dependent, it is represented by image data. A deep learning model is developed to find a relationship between the two image data sets which are the microstructure and the relaxation moduli. The deep learning model is constructed based on a convolutional neural network (CNN). Both the homogenization and the inverse homogenization problems can be solved by the proposed deep learning model. A microstructure of viscoelastic composite with desired relaxation moduli can be designed by utilizing the trained deep learning model.

Physical models and reduced order models augmentation with data for physics-informed machine learning in real-world applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

REAL-TIME DEFECT DETECTION IN STRUCTURAL COMPONENTS: AN INTEGRATED MACHINE LEARNING-ENHANCED MODEL ORDER REDUCTION AND SEARCH ALGORITHM APPROACH

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ABSTRACT

Mechanical defects resulting from handling, transportation, and manufacturing significantly impact a material's response to applied loads. Conventional numerical simulations for defect detection face challenges due to computational expenses. In response, our study introduces an innovative methodology seamlessly integrating a Machine Learning-enhanced Model Order Reduction technique with a dedicated search algorithm for efficient defect detection.

The machine learning-enhanced technique incorporates Proper Orthogonal Decomposition (POD) for model order reduction and employs Random Forest for Machine Learning, allowing versatile training for diverse defect scenarios. This non-intrusive approach facilitates real-time displacement prediction with varying parameters. The combined use of model order reduction and the search algorithm, adaptable to defect sizes, locations, and degrees, enables on-the-fly determination of displacements in real-time.

This novel methodology represents a significant advancement in structural health monitoring, providing a swift and online approach to defect detection. Its real-time capabilities empower efficient structure management by facilitating the timely identification and response to hidden defects, ultimately enhancing overall structural integrity.

Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADVANCING DIRECTED ENERGY DEPOSITION SIMULATIONS THROUGH OPERATOR LEARNING-BASED REDUCED ORDER MODEL DEVELOPMENT

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ABSTRACT

The directed energy deposition (DED) process, a widely utilized additive manufacturing technique, involves intricate physical mechanisms that remain insufficiently understood to this day. Computational tools hold promise for unraveling this complexity and facilitating nondestructive performance evaluations of manufactured parts. A critical challenge in this field lies in the significant space and time scale differences between realistic DED processes and numerical simulations. Current direct numerical simulation approaches struggle to encompass all the intricate physics phenomena across multiple scales within a timeframe comparable to real DED processes. To address this gap, our work focuses on the development of reduced-order models (ROMs) for DED [1-2], based on the Multiphysics Object-Oriented Simulation Environment (MOOSE) framework [3-4]. Notably, machine learning (ML) techniques, which are becoming especially popular in ROM creation, carry the potential for quick, accurate predictions across a diverse range of problems. In the present study, we specifically explore utilization of the operator learning (OL) approach, which enables the learning of a family of differential equations across a broad spectrum of process and material parameters. In addition, we employ deep neural networks (DNNs) and physics-informed neural networks (PINNs) to create ROMs. A comparative analysis of their performance sheds light on the efficacy of these ML approaches in enhancing the speed and accuracy of simulating the DED process. The findings contribute to bridging the gap between realistic DED processes and numerical simulations, showcasing the potential of ROMs and ML techniques to advance our understanding and accelerate simulations in DED.

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Computational and analytical advances in nonlocal modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FULLY ANISOTROPIC MATERIAL MODELS IN ORDINARY STATE-BASED PERIDYNAMICS

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ABSTRACT

The need to optimise the use of resources and adapt the performance of materials to the specific requirements of applications has promoted the adoption of materials with anisotropic properties. Several engineering sectors, such as structural engineering, aerospace and bioengineering, are taking advantage of this possibility. Therefore, within the framework of classical continuum mechanics, appropriate constitutive laws have been developed to model the mechanical behaviour of these materials [1]. Unfortunately, the need to simulate material failure and damage propagation requires the adoption of alternative theories to the classical one. Peridynamics (PD) theory [2] has proven particularly effective in simulating the propagation of discontinuities such as cracks, therefore it is crucial to develop constitutive laws for anisotropic materials in PD. For that purpose, the use of bond-based PD is limited by the inherent restrictions on the values of the mechanical properties that can be simulated [2], while the use of non-ordinary state-based PD [3] requires the adoption of strategies to mitigate the problem of zero-energy modes. Ordinary state-based PD, on the other hand, does not suffer from the limitations of the other PD versions. We therefore propose an ordinary state-based PD formulation capable of modelling the linear elastic behaviour of fully anisotropic materials in both 2D and 3D. With the developed strategy, all components of the elasticity tensor of classical continuum mechanics expected for anisotropic materials can be effectively reproduced within the PD framework. To achieve this, two distinct micromoduli were introduced that depend on the orientation of the bonds and were defined to correspond to the classical mechanical properties in the case of an infinite body subjected to homogeneous deformation. The new formulation was applied in several 2D and 3D examples to demonstrate its effectiveness and accuracy.

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Scientific deep learning
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HYBRID DEEP LEARNING APPROACHES FOR DYNAMIC ANOMALY DETECTION IN BIO-FET BASED BIO-CYBER INTERFACES

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ABSTRACT

The Internet of Bio-Nano Things, or IoBNT, is a new paradigm that uses biological transceivers that are nanoscale (~1-100 nm) to gather in vivo signaling data from the human body. The healthcare practitioners are then informed of this information through the Internet. Targeted drug delivery to previously unreachable areas of human tissue is made possible by bio-nano-things (BNT), which allow external actuation of in-body molecular communication (MC). These BNTs are linked to an external ex vivo environment, like the Internet, through bio-cyber interfaces, forming an in body bio-nano network via chemical diffusion channels.

Because of its affordability and non-intrusive design, Bio-Fet bio-cyber interfacing (BFI) has showed promise in the field of IoBNT systems. However, because Internet access exposes interfaces to external threat vectors, the installation of Bio-Fet BFI generates security risks. For effective mitigation, accurate characterization of aberrant BFI traffic patterns becomes essential. Current machine-learning (ML) techniques for anomaly identification, which frequently depend on manually designed features, are constrained by the intricacies of the connections between BFI traffic attributes and their parameters.

In order to overcome these challenges, this work investigates the use of deep learning (DL) methods, which enable dynamic and scalable feature engineering for the purpose of differentiating between typical and abnormal BFI traffic. After a thorough validation process on the created dataset utilizing singular and multi-dimensional models, our hybrid convolutional and recurrent ensemble (CNN + LSTM) outperformed other deep and shallow structures with an accuracy of upto ~83.56%. The incorporation of a hybrid deep learning network enabled the automated extraction of normal and temporal characteristics from BFI data, hence obviating the necessity for manual feature selection and crafting for precise prediction.

Finally, this work advocates for the integration of emerging non-Von Neumann architectures for real-time anomaly detection and suggests implementing the extracted best classifier in traditional intrusion detection systems. This research advances the development of safe and effective IoBNT systems by emphasizing the scalable and dynamic properties of DL algorithms, especially when it comes to Bio-Fet bio-cyber interfacing.

Modeling and inverse design of architected materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFICIENT DESIGN AND SIMULATION OF NONLINEAR METASTRUCTURES USING MAXIMALLY-LOCALIZED WANNIER FUNCTIONS

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ABSTRACT

Elastic wave propagation in typical MEMS structures (made of e.g., Silicon or Silicon Nitride) has an extremely low energy dissipation, which makes these structures a promising candidate for metamaterial-based passive (or near-zero power) neuromorphic information processors. However, designing elastic structures that perform computations is a formidable challenge. The reason is that neural networks require a massive number of neurons (in this case, implemented with nonlinear resonators), reaching the limits of direct optimization based on the Finite Element Method. This requires the development of new methods capable of efficiently modelling the nonlinear response of elastic metamaterials.

In this research, we have developed a new model order reduction technique based on the concept of Wannier functions – linear combinations of lattice eigenmodes that are maximally localized at each resonator site. This method draws inspiration from the basis functions used in Density Functional Theory modelling of material responses. In comparison with other reduced order models, this method has two significant advantages: The first key benefit is the sparsity of the reduced nonlinear tensors. The second is the local dependence of each model parameter in one oscillator and its neighborhood, which allows us to extract the effective parameters by repeatedly simulating small clusters of sites instead of the entire lattice. The combination of these two properties allows us to effectively simulate highly complex, non-periodic metamaterials in linear time with the number of sites. In addition to representing the system dynamics using a basis of maximally-localized functions, we use the quadratic manifold technique to statically condense higher-order modes (such longitudinal displacements arising from to geometric nonlinearity), without significantly increasing the computational cost.

The method works in both static and dynamic regime and can capture non-trivial properties such as buckling. We will illustrate the capabilities of our method by designing functional metamaterials (such as logic gates and topological insulators) and validating their performances against high-fidelity simulations.

Recent advances in high-order methods for computational fluid dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A P-ADAPTIVE IMPLICIT SHOCK TRACKING METHOD FOR HIGH-SPEED VISCOUS FLOWS

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ABSTRACT

Shock tracking or shock fitting, where the computational mesh is moved to align mesh element faces with discontinuities, represents them perfectly with the inter-element jump in the solution basis without requiring additional stabilization when addressing shocks. In our previous work, we introduced an implicit shock tracking framework that discretizes conservation laws on a mesh without knowledge of discontinuities and solves a PDE-constrained optimization problem over the discrete solution variables and nodal coordinates of the mesh. A Discontinuous Galerkin (DG) discretization of the governing equation is applied and implicit tracking is formulated as an optimization problem constrained by the DG residual to endow the method with desirable properties of DG: consistency, conservation, and stability. The optimization problem is solved using a sequential quadratic programming method that simultaneously converges the mesh and flow solution to their optimal values.

In this talk, we present a p-adaptive implicit shock tracking method aimed at solving steady and unsteady high-speed viscous flows. The polynomial degree is adapted used an indicator based on the enriched residual, which tends to increase the polynomial degree within shocks and boundary layers. A series of shock-dominated numerical experiments demonstrate the potential of the method to efficiently produce accurate solutions to these challenging problems.

Machine learning methods for multiscale and multiphysics material modeling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MICROSTRUCTURE-BASED FINITE ELEMENT MODELING OF THE STRAIN-RATE-DEPENDENT MECHANICAL BEHAVIOR OF ADDITIVELY MANUFACTURED ALUMINA CERAMICS: TOWARDS COUPLING MULTISCALE MODELING AND DATA-DRIVEN APPROACHES

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ABSTRACT

This study develops a microstructure-based finite element (FE) model to predict the strain-rate-dependent mechanical failure behavior of additively manufactured (AM) alumina ceramics towards coupling with machine learning approaches for the development of a data-driven model. AM alumina was first micro-structurally characterized and the data (i.e., grain size distribution, grain crystallographic orientations, and void volume fraction) was used to generate polycrystalline-based representative volume elements (RVEs) of the material. To account for the transgranular failure mechanism, the grains were constitutively modeled by the JH2-V (i.e., a viscosity regularized form of the Johnson–Holmquist-II (JH2) model) model where the strain-rate-dependent behavior of ceramics is accounted for, and this model was implemented by a VUMAT subroutine in Abaqus/Explicit solver. The interfaces between the grains were modeled by the bi-linear cohesive zone model (CZM) approach to account for the intergranular failure mechanism. The microstructure-informed FE model was validated by experimental data derived from rate-dependent testing coupled with ultra-high-speed imaging (e.g., stress-time histories and fracture processes). Here, the evolution history of the failure mechanisms in the model was quantified by the fraction of fully damaged entities (i.e., elements or interfacial nodes) to provide a better understanding of the initiation and growth of the failure in the material. Next, the validated FE model was leveraged to study the effect of microstructural features (e.g., void volume fraction, void size, and interface properties) on the macro scale response of the AM alumina. The current microstructure-based FE model will be exercised to generate datasets for the training and validation of an artificial neural network (ANN) that correlates the mechanical properties of the material (e.g., strength) at the macroscale to the microstructure and strain rate. Such a computationally efficient surrogate model has great potential to be utilized for accelerating the design and optimization of better-performing AM ceramics as future materials.

Advances in computational biomechanics and mechanobiology
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPLORING BIOTRANSPORT IN A POROELASTIC MODEL OF HUMAN VOCAL FOLDS

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ABSTRACT

The aim of this study is to analyze the role of porous media in modeling the flow and oxygen transport in the context of human phonation modelling. Poroelastic models are suitable to characterize the biomechanics of the vocal folds as their tissue are composed of dispersed cells separated by connective voids which allow for the flow of nutrients. Considering the interactions between the airflow through the larynx and the deformation of the fluid-saturated poroelastic vocal folds and integrating this fluid-structure interaction (FSI) coupling with mass transport, improves our ability to compute local changes in oxygenation and perfusion within the tissue. Previous experimental observations report contradictory relationships regarding the effects of phonation on the flow within the tissue and the associated oxygen partial pressure. It has been hypothesized that permeability may influence tissue oxygenation, which corresponds with dysfunctions such as hypoxia and localized lesions.
Our prior research studied the liquid dynamics within the vocal folds by considering a biphasic model for the tissue. In this current study, we aim to combine our FSI-porous vocal fold model with a mass transport model to investigate the association of interstitial flow with oxygen transport within the vocal fold, as well as to explore the interplay between permeability and interstitial liquid velocity within the porous structure. A multiphysics coupled mass transport-FSI computational model by considering transient Navier-Stokes equations for the glottal airflow, Brinkman equation for the interporous flow, and advection-diffusion-reaction equation for oxygen transport is developed. Additionally, the tissue dynamics is modeled using the Biot system of equations for a poroelastic medium. This integrated fluido-chemical framework can numerically simulate the complex flow fields, mechanical stresses, and oxygen concentrations. To analyze the significance of physiological features behind biotransport, selected parameters such as tissue porosity and permeability and lung pressure are varied, and coupled biomechanical simulations of transient glottal aerodynamics, vocal fold tissue dynamics, interstitial fluid dynamics, and oxygen flow are performed. The simulation results focusing on the interstitial velocity streamlines and oxygen concentration contours are measured and analyzed. It is found that oxygenation is directly related to permeability, and not noticeably affected by lung pressure. It is also found that interstitial fluid flow is linearly proportional to lung pressure and exponentially related to permeability. Results facilitate a better understanding of the mechanisms behind the role of poroelasticity on biomechanics and biotransport in phonation models.

Trustworthy multi-fidelity and data-driven models for computational applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CONSTRAINED COST-AWARE MULTI-FIDELITY BAYESIAN OPTIMIZATION

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ABSTRACT

Bayesian optimization (BO) is a widely used technique for finding materials with unprecedented properties. However, relying solely on expensive high-fidelity (HF) sources can inflate optimization expenses in complex scenarios. To address this challenge and incorporate known and unknown constraints, we introduce a novel constrained cost-aware multi-fidelity BO (C2-MFBO) framework which a few novelties. Firstly, it uses manifold-embedded Gaussian process (GP) for emulation which handles mixed input spaces and models source-dependent noise and global trends. Secondly, it leverages a composite acquisition function (AF) that quantifies the information value of high- and low-fidelity sources differently and also accommodates source-dependent constraints. Through analytical and real-world examples, we will demonstrate the benefits of our approach which is publicly available via the GP+ package in Python.

Computational damage and fracture mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL CRACK PATH PREDICTION IN ANISOTROPIC INHOMOGENEOUS MATERIALS

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ABSTRACT

Materials and manufacturing processes are being further developed to meet increasing demands on design and energy efficiency. As a result of the addition of additives to composites or the deformation and heat treatment of metals, these materials exhibit anisotropic mechanical properties. Fracture mechanics, with loading quantities such as the J-integral, complements stress analyses with the FEM in the context of least conservative component design. Due to path independence, the J-integral offers the advantage that numerical inaccuracies at the crack tip are avoided. Furthermore, it is suitable for accurately predicting crack deflection and crack paths [1]. The classical J-integral criterion implicitly takes into account the elastic anisotropy, but not the anisotropy of the fracture toughness. The latter, however, has a considerable influence on the crack deflection behavior regardless of its origin, e.g. in fiber composites [2] or in formed aluminum alloys due to the textures of the grain structure [1]. Therefore, a modified anisotropic J-integral criterion is introduced for a reliable prediction of crack paths.

The crack deflection behavior of different materials varies significantly depending on the degree and shape of the anisotropy. In addition, depending on the manufacturing process, materials exhibit local inhomogeneity of anisotropy. Therefore, stochastic aspects must be taken into account in modeling and simulation [2]. A special case of anisotropy is given by imperfect interfaces or bimaterials, as the crack growth resistance within an interface and that of adjacent materials differ in general. In the context of cohesive zones, oftentimes being applied for interface modeling, the J-integral requires an adaptation involving a cohesive interface contour integral, whereby its numerical implementation, based on inaccurate data of field quantities on the crack boundaries of the cohesive zone [3], represents a challenge.

This work aims at demonstrating the influence of various sources of anisotropy on crack deflection behaviors in the context of crack growth simulations. The focus is on bifurcation phenomena, stochastic aspects and the application of the J-integral and its related deflection criterion to interface-matrix crack transition problems. Selected results are finally compared to experiments.

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Architected materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CHALLENGES AND OPPORTUNITIES IN DESIGNING STIMULUS-RESPONSIVE ARCHITECTED MATERIALS WITH HIGH WORK CAPACITY

Phani Saketh Dasika[1], Haohuan Xu[1], Yunlan Zhang[2] and Pablo Zavattieri[1]*

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ABSTRACT

The field of architected materials, fueled by advances in additive manufacturing, has enabled new materials with new and improved emerging properties. More recent efforts have recently focused on a new family of stimulus-responsive architected materials and structures that are designed to exhibit dynamic and programmable behavior as they respond to external stimuli, such as temperature, light, pH, mechanical stress, etc. making them suitable for sensors, actuators, drug delivery systems, among others. In this work, we introduce new concepts that will enable us to explore new spaces in the material design maps. In particular we are interested in applications related to morphing, actuation, self-deployment/-reconfigurability where relatively high forces are required. Combining insights from previous works on architected material analogs for shape memory alloys and bioinspired materials, we integrate concepts not extensively explored before, with a strong focus on improving the work capacity of the architected material. To mimic the actuation capabilities of traditional shape memory materials, the challenge lies in understanding the forces involved in the mechanisms that take place at the unit cell and how these forces translate into the emergent work capacity of the material. Achieving this with a simple combination of two polymeric materials has been shown to be particularly challenging. In this talk, I will explain the conceptual framework and how these principles are put into practice through architected materials in such a way that these materials can be used for actuation with a focus on improving their work capacity. We will discuss the complexities of ensuring desired stiffness in unit cells at low/high temperatures and explore innovative bistable/monostable designs, crucial for distinguishing our work in smart architected materials.

Modern structure-preserving methods for PDEs
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DE RHAM COMPATIBLE NEURAL NETWORK FEM

Marcello Longo[1], Joost Opschoor[1], Nico Disch[2], Christoph Schwab[1] and Jakob Zech[2]*

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ABSTRACT

Recent years have seen the emergence of methodologies that approximate PDE solutions via neural networks (NNs). These methods minimize a 'physical' loss, such as the PDE residual or the corresponding energy, thereby representing the PDE solution as a NN output. Consequently, understanding the conditions under which network architectures can represent standard, variationally correct, and structure-preserving finite element spaces from numerical analysis is of considerable interest. In this talk, we construct exact NN emulations of all lowest order finite element spaces within the discrete de Rham complex. These include piecewise constant functions, continuous piecewise linear functions, the classical "Raviart-Thomas element," and the "Nédélec edge element," thereby covering a wide range of problems in computational mathematics. Our construction and NN architecture generalizes previous results in that no geometric restrictions on the regular simplicial partitions of the domain are required for NN emulation.

Catastrophic failure mechanics and numerical modelling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STUDY ON IRRADIATION THERMO-MECHANICAL BEHAVIOR OF SURROGATE FCM PELLETS

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ABSTRACT

Fully ceramic microencapsulated (FCM) fuel has good radiation stability and fission product retention ability under accident conditions, which is considered a momentous direction for the development of accident-tolerant fuel (ATF). FCM fuel pellets are composed of TRISO particles randomly dispersed in a SiC matrix, in which TRISO have multi-layered microstructure, including a fuel kernel, a porous carbon layer (buffer), an inner pyrolytic carbon layer (IPyC), a SiC layer, and an outer pyrolytic carbon layer (OPyC). To improve the economy and safety, it is necessary to conduct in-depth research on the irradiation thermo-mechanical behavior of FCM fuel pellets. For individual effect testing and development of the consolidation process, the Oak Ridge National Laboratory replaced the UO2 kernel with ZrO2 to fabricate the surrogate FCM pellets and carried out the irradiation experimental study on them. Surrogate FCM pellets have complex thermo-mechanical behavior under the irradiation environment. The irradiation effect of each part in the pellet is perfectly considered. A three-dimensional mechanical constitutive, calculation method and program are developed based on the theoretical framework of large deformation. According to the experimental result of the interface cracking of the kernel/buffer, the cohesion model, calculation method, and program are developed. The interface cracking numerical simulation in the irradiation experiment is realized. The results show that: i) The interface cracking can occur under very small irradiation doses. The predicted swelling and internal microstructure information of the pellet are in good agreement with the experimental results; ii) The anisotropic irradiation shrinkage of the buffer skeleton has a dominant influence on the thickness change of buffer and the interface gap width, and the skeleton irradiation creep also has an important influence on the size change, porosity, and skeleton stress evolution. In the simulation of the irradiation thermo-mechanical behavior of FCM pellets, it is critical to use a volume growth strain model that takes into account the contribution of irradiation shrinkage and creep of the buffer skeleton. iii) The first principal stress of the SiC layer first increases with the increase of fast neutron fluence, reaches the maximum value at low fluence then decreases with the increase of fast neutron fluence. The experimental observation after irradiation found that there was no damage in the SiC layer, indicating that its tensile strength is particularly high (over 1800 MPa). Thanks for the support of National Natural Science Foundation of China (Nos.12132005,12135008,12102094,), and the support from Shanghai Sailing Program (21YF1402200).

Advances in multi-scale, multi-material, and multi-component Topology Optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

IMPOSING MANUFACTURING CONSTRAINTS USING POLYGONAL PRIMITIVES PARAMETRIZATION

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ABSTRACT

Topology optimization has been proven to result in efficient designs in many engineering applications. An ongoing challenge remains in realizing optimized design, where manufacturing requirements necessitate manual adjustments and corrections. To deal with this challenge in density-based optimization, where the geometry is implicitly defined, manufacturing constraints are considered through different schemes of filtering and projection. Examples of such constraints include length-scale control, overhang constraints, machining constraints and others. Feature mapping approaches, on the other hand, are characterized by explicit geometrical parametrization, where geometrical primitives are explicitly parametrized and projected on a fixed background mesh. This explicit parametrization facilitates convenient imposition of geometrical constraints. However most existing studies are limited to shapes that have analytical singed distance function (SDF), and thus offer limited geometrical freedom. Recently, a new polygonal primitive (PP) was introduced that can have any number of sides, can form both convex and non-convex shapes, thereby offering great geometrical freedom. At the core of the formulation of the PP is an approximated SDF that is analytical and explicit in terms of the vertices' coordinates.
In this study, we leverage the rich and explicit shape parametrization, as well as the explicit SDF of the PP to impose different manufacturing constraints. The results show that manufacturing constraints that would have been difficult to impose using density-based optimization or traditional feature mapping approaches can be readily handled with polygonal primitives.

Recent advances in computational fracture mechanics and failure analysis
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A PHASE-FIELD FRACTURE MODEL FOR BRITTLE MATERIALS SUBJECTED TO THERMAL SHOCKS

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ABSTRACT

The modeling of brittle materials fracturing under thermal shocks presents a number of challenges. Shock conditions are characterized by rapid temperature increases, such as from room temperature to over 1000 Celsius degrees in tens of microseconds. This can give rise to large thermal strains and stress gradients that exceed the strength of the material, eventually giving rise to crack formation. This study looks to reproduce a series of fracture tests for sintered ceramics subjected to thermal shocks, with the aid of a thermomechanical model coupled with phase-field fracture. In particular, to model the fracturing in the bulk material, a phase-field model that explicitly incorporates material strength as a nucleation criterion is adopted. We will show that with a controlled perturbation to the system, the model is able to reproduce various experimental observations.

Immersed-boundary variational methods: Theory, data structures, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMPRESSIBLE EULER FLOW COMPUTATIONS AND AERODYNAMICS USING THE SHIFTED BOUNDARY METHOD

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ABSTRACT

In this talk we present the Shifted Boundary Method (SBM) for inviscid compressible flows on complex and deforming domains with aerodynamic applications. The Shifted Boundary Method belongs to the class of unfitted finite element methods. It reformulates the original boundary value problem over a surrogate (approximate) computational domain that does not have to be conformal to the true geometry; and accuracy is maintained by modifying the original boundary condition using Taylor expansions. Because SBM avoids integration over cut cells, it does not suffer from small time-step issues and allows efficient explicit time integration. Previously the SBM has been applied to solve the Poisson equations, Stokes flow equations, and viscous incompressible flows on complex domains, and in this talk we detail the derivation of SBM for more complex wave structures for Euler equations.

In addition to the general methodology derivation and numerical verification, we also discuss the advantages the SBM offers in avoiding spurious numerical artifacts in two scenarios: (a) when curved boundaries are represented by body-fitted polygonal approximations and (b) when additional condition needs to be enforced at a geometrical singularity, such as the Kutta condition at the trailing edge of an airfoil. Lastly, we investigate how these advantages enable SBM to perform efficient and reliable aerodynamics computations to problems like flow past a flapping airfoil.

Uncertainty characterization and error control to enable predictive simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DATA-DRIVEN UNCERTAINTY QUANTIFICATION AND PREDICTION FOR MODELS WITH HIGH-DIMENSIONAL DEPENDENT PARAMETERS

Xiaoshu Zeng[*1] and Roger Ghanem*[1]

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ABSTRACT

Complex physical systems often involve high-dimensional parameter spaces, particularly when dealing with uncertainty quantification (UQ) and response prediction. Exhaustively exploring the entire parameter space is impractical due to the computational cost associated with accurate high-resolution models. In such scenarios, UQ and prediction tasks encounter two significant challenges: the curse of dimensionality and the intricate dependency structure among the parameters. Recent work by the authors introduced a data-driven Projection Pursuit Adaptation (PPA) method within the framework of polynomial chaos expansions. This method utilizes independent Monte Carlo samples to identify an optimal low-dimensional parameter space adapted to the quantities of interest. By reducing parameter dimensionality, PPA efficiently constructs accurate surrogate models for UQ and prediction, even with a limited number of samples. In this study, we extend PPA to handle dependent parameters. While Rosenblatt transformation is commonly employed to decouple input parameter dependencies, it necessitates knowledge of the joint parameter distribution, which can be data-intensive to estimate. Therefore, we propose using multivariate Regular Vine (R-vine) copulas to capture parameter dependency structures, which are typically more accessible to estimate from available data. R-vine copulas contain the necessary joint distribution information and can be integrated into the Rosenblatt transformation to decouple dependent parameters. We combine R-vine copulas with the PPA method to establish a unified data-driven framework for surrogate modeling of complex physical systems with high-dimensional dependent parameters. This approach relies on a minimal number of independent Monte Carlo samples to construct accurate UQ and prediction models. The method has been tested on both a borehole model and a space structure, demonstrating its significant potential in accurate surrogate modeling.

Modeling friction and wear
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FRICTIONAL CONTACTS BETWEEN ROUGH GRAINS WITH FRACTAL MORPHOLOGY

Chongpu Zhai[*1], Deheng Wei[2] and Hengxu Song[34]*

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ABSTRACT

Friction depends on geometries of both surfaces of a contact pair, yet numerical or analytical studies involved in two rough surfaces are limited. In this study, we revisit the Cattaneo-Mindlin problem for the contact between two elastic or elasto-plastic spheres with isotropically fractal roughness generated based on ultra-high degree Spherical Harmonics. Transverse contacts are simulated by finite element method (FEM), which is validated by the extended Cattaneo-Mindlin solution to full slip regime for smooth sphere contacts. Gigantic parameter studies, including material properties, intrinsic friction coefficient, normal contact distance, relative roughness, fractal dimension, and wavelength range, in the FEM simulations show that: (1) the newly extended Cattaneo-Mindlin solution can approximately predict the macro contact response between two rough spheres except for extremely high relative roughness and narrow wavelength range; (2) departures induced by roughness of macro normal and frictional forces from smooth sphere contacts can be neutralized by plasticity, deep normal contact interference, and higher intrinsic micro friction coefficient; and (3) considering the realistic values of the two factors adequately quantifying the multi-scaled rough grain topology, fractal dimension impacts frictional contacts less than root mean square roughness. The main cause of these phenomena can be credited to the underlying microscale contact information; distributions of contact areas and stresses and their evolutions provide concrete evidence of the observed behaviour. Our results provide a pathway for applying computational contact mechanics to many geophysical fields involving frictional contacts, such as the asperity model in earthquake engineering and the mechanics of granular materials.

Nanomechanics and nanoscale thermal transport for new materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TENSION-COMPRESSION ASYMMETRY OF NICKEL ALLOY VIA ATOMISTIC SIMULATIONS

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ABSTRACT

Nickel-based single crystal alloys exhibit significant tension-compression asymmetry during service [1,2], and a thorough analysis of their underlying mechanisms is crucial for optimizing its design and predicting its service performance. In this study, the collective variable hyperdynamics (CVHD) method was employed to investigate the vacancy diffusion in nickel under different pressures and temperatures through molecular dynamics simulations [3]. Our simulation revealed that the vacancy diffusion rate in nickel decreases as hydrostatic pressure increases. When uniaxial stress is applied, both tension and compression stress states accelerate the total diffusion rate and introduce anisotropy in diffusion. Additional investigation indicates that size significantly influences its mechanical properties. The initial dislocation evolution during the elastic stage and the dislocation non-uniformity caused by lattice rotation during plastic flow play crucial roles in tension-compression asymmetry.

DEVELOPMENT OF GPU ACCELERATED KINETIC MODELING CODES IN FUSION PLASMA PHYSICS AND GAS DYNAMICS

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ABSTRACT

Kinetic theory studies the physical system from the microscopic descriptions of atoms, molecules, ions, electrons, and their interactions. Kinetic modeling represents a more accurate description compared to the continuum approach. The governing equation of kinetic theory is the Boltzmann equation. To solve this integro-differential equation accurately and efficiently, particle-based simulation methods are being widely used in kinetic modeling. Owning to their unique properties, particle methods can largely benefit from the advancement in GPU accelerated high performance computing [1, 2].

We discuss recent work developing two GPU accelerated particle simulation codes, XGCm [3] and Comet. XGCm is a gyrokinetic particle-in-cell (PIC) code used in fusion plasma physics. Comet is a direct simulation Monte Carlo (DSMC) code used in hypersonic flow and rarefied gas dynamics, including micro and nanoscale flows. Despite the distinct application areas, they are rooted in the same kinetic modeling framework. Both codes use distributed unstructured mesh and mesh-centric data structure for particle operations. They employ several open source libraries to interact with GPUs and perform parallel operations, including Kokkos, Omega_h, Cabana, PUMIPic, and PETSc.

We first briefly discuss the numerical methods and algorithms used to perform particle operations on the GPUs. We then present code validation studies. In XGCm, the circular geometry cyclone base case is used and the calculated turbulence growth rate shows excellent agreement with existing simulation results. In Comet, simulation results of hypersonic rarefied gas flows are compared with existing experimental data. Finally, we show the parallel performance of the two codes, particularly the excellent weak scaling of XGCm on Summit supercomputer at the Oak Ridge National Laboratory.

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ELECTROMAGNETIC COILGUN LAUNCH OF HIGH-TEMPERATURE PROJECTILE CONSIDERING THERMAL EFFECT

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ABSTRACT

Blade containment of turbine engines is a long-term concern. The blades are always exposed to high temperatures and high energy, which causes fatigue damage to the material and produces high-velocity debris impacting the engine casing. The casing needs to contain debris to prevent it from penetrating, otherwise it will be a serious safety hazard to the flight.

Most studies on blade containment are ballistic impact tests with air guns. The combination of the projectile and the sabot needs to cling to the gun barrel during the air gun launch. If a high-temperature projectile is launched, it will produce a strong heat conduction with barrel, which will affect the working life of the barrel. Moreover, it takes a long preparation time for air gun launch, which leads to a long cold contact time and a large heat loss of the high-temperature projectile. Therefore, it is difficult to launch projectiles at high temperature, and the impact resistance of casing at high temperature is mostly tested only by heating the target.

The idea of loading a high-temperature projectile using an electromagnetic coilgun was proposed. The electromagnetic coilgun is quite different from an air gun because of its short preparation time, high launch efficiency and accuracy, and no contact between the projectile and the gun barrel. Therefore, a preheated high-temperature projectile can be dropped into the barrel through heat insulation, and then directly launch. Heat is lost during dropping and launching, but the current induced by the conductors in electromagnetic fields also causes thermal resistive of the projectile, which can be calculated separately in theory. In this paper, a theoretical model of the dynamic response of the projectile during electromagnetic launch is established, and the movement and temperature changes of the projectile are analyzed. The theory can provide technical support for electromagnetic coilgun launch of high-temperature projectiles. On this basis, the feasibility of carrying out the research on high-temperature blade containment based on electromagnetic coilgun launch is prospected.

Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATION OF MATERIAL POINT METHODS TO OBJECTS WITH COMPLEX GEOMETRIES

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ABSTRACT

We use the material point methods (MPM) to overcome many difficulties related to numerical simulation of objects with complex geometries subjected to extreme deformations and stresses. These issues include complex geometries of 3-D printed materials, mesh or material point generation from CT-scanned images, and distortion of elements in typical Lagrangian methods. Different form many other mesh-based methods, in MPM we can use positions of material points to accurately represent the location and shape of an object. The material points can be generated from stereolithography (STL) files commonly used in advanced manufacturing and computer aided design applications. The background mesh in material point method calculations is not required to be body conforming. The efficiency, accuracy, convergence, and convenience of the method are illustrated using examples.

For the pre- and post- processing of the numerical results, we benchmark the significant efficiency improvements of a new material point generation method and then discuss the presentation of numerical results using the STL file format on material surfaces. Traditionally, the material points are generated based on the computational meshes. With the new efficient material point generation technique, the material points can now be generated independent of the mesh. This new capability causes a new issue related to different numbers of initial material points in adjacent cells. An efficient numerical algorithm has been developed to address the issue. With the algorithm, we will also show the freedom gain of using material point methods.

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Multiscale, multifield, and continuum-discontinuum analysis in geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COUPLED HYDRO-THERMO-MECHANICAL MODELING CONSIDERING PHASE TRANSITION FOR SC-CO2 FRACTURING IN FRACTURED ROCKS

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ABSTRACT

Abstract: Supercritical carbon dioxide (Sc-CO2) fracturing is a developing fracturing technology in the unconventional reservoir stimulation due to its potential to increase production, reduce water requirements, and minimize environmental impacts. With the injection and transport of cold CO2 in geological fractured reservoirs, the elevated reservoir pressure and thermal effects mutually lead to rock deformation and fracture propagation. Once the fracture dynamically propagates, a large void volume would be instantly created causing Sc-CO2 expansion at the fracture tip and inducing the phase transition within the fracture. The phase transition would have a significant influence on the distribution of pressure and temperature, as well as the fracture deformation. However, the phase transition effect is commonly neglected within the fracture in previous numerical studies.

In this study, a coupled hydro-thermal-mechanical model considering phase transition in fractured media was developed to investigate multi-phase flow, heat transport, the CO2 phase transition as well as the fracture deformation and propagation during Sc-CO2 fracturing process. The Span-Wagner equations and the transport equations were introduced to determine the variations of CO2 properties. The modified specific heat capacity, as the characteristic quantity of phase transition, was used to describe the interphase heat transfer. Mixture fluid flow in the rock matrix and fracture was governed based on the modified Darcy law. Heat exchange between fluid and rock matrix obeyed the local thermal non-equilibrium principle. In addition, the effective stress theory and thermal strain effect were taken into account in the stress equilibrium equation of porous rock matrix. The damage of element nodes was judged by the maximum tensile stress failure criterion and Mohr-Coulomb failure criterion according to the continuum damage mechanic model.

The commercial software COMSOL and MATLAB were coupled to solve the multi-field equations. The accuracy and reliability of the numerical method are evaluated and confirmed by the published results. The spatiotemporal evolution of CO2 phase state within the fracture was revealed, and the effects of SC-CO2 phase transition on the coupling characteristics of temperature field, pressure field and deformation field were discussed.

This developed numerical framework and analysis results are expected to provide insight into the effect of phase transition during SC-CO2 fracturing, thereby laying theoretical base for evaluating fracture morphology and fracturing effect.

Key Words: Sc-CO2 fracturing, phase transition, hydro-thermo-mechanical coupling

Modeling, optimization and computational analysis of metamaterials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

BANDGAPS IN ACOUSTIC METAMATERIALS: DESIGN AND UNCERTAINTY QUANTIFICATION INCLUDING STOCHASTIC GEOMETRIC DEFECTS AND MATERIAL PROPERTIES

Han Zhang[*1], Rayehe Karimi Mahabadi[1], Cynthia Rudin[1], Johann Guilleminot[1] and Catherine Brinson[1]*

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ABSTRACT

Acoustic metamaterials are a subject of increasing study and utility. Through designed combinations of geometries with material properties, acoustic metamaterials can be built to arbitrarily manipulate acoustic waves for various applications. Despite the theoretical advances in this field, however, acoustic metamaterials have seen limited penetration into industry and commercial use. A significant bottleneck is the difficulty of manufacturing the required intricate geometries and the sensitivity of metamaterial designs to material batch variability and manufacturing defects. Capturing the effects of stochastic material properties and geometric defects requires empirical testing of manufactured samples, which is prohibitively expensive with high precision requirements or with an increasing number of input variables. Through the application of uncertainty quantification techniques, sampling needs can be greatly reduced for characterizing acoustic meta- material dispersion characteristics. For the case of stochastic material properties and geometry, two to three orders of magnitude sampling reductions were achieved in a 7D input space scenario with polynomial chaos expansion and spectral projection, combined with a novel method of encoding geometric defects with a scalar parameter.

Remarkably, this reduction in sampling was possible while preserving accurate output probability distributions of the metamaterial performance characteristics (bandgap size and location). Ongoing work focuses on enhancing metamaterial design iteration efficiency and inverse design capabilities by leveraging the latest advances in deep learning techniques.

New trends in topology optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

UNSUPERVISED-MACHINE-LEARNING ASSISTED TOPOLOGY OPTIMIZATION FOR MULTIFUNCTIONAL STRUCTURE WITH BIONIC STRUCTURAL GENE

Heng Zhang[*1], Sen Kong[1] and Xiaohong Ding[1]*

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ABSTRACT

As we know many bionic structures show excellent multifunctional mechanical performance, for example, the honeycomb structure has better high stiffness lightweight, and good energy absorption performance, and the bone trabecula also shows similar performance. To integrate these bionic structure genes into the structural topology optimization. This study proposes an unsupervised-machine-learning assisted new topology optimization method for multifunctional structure design[1]. To embed the bionic structural gene into the design, a neural style transfer technique is adopted for measuring and generating the prior knowledge from a reference bionic structure image with the concerned functional gene. The new structure obtained by combining the traditional topology-optimized structure and the given biological structure features not only maintains the original mechanical performance of the topology-optimized structure, but also obtains the special performance of the biological structure, for example, energy absorption. Firstly, the pre-trained VGG19 convolutional neural network(CNN) is selected as a feature extraction tool[2], and the CNN is used to extract and quantify the structural features from biological structures and topology-optimized structures. The total loss function is established by style and content loss. Secondly, taking the total loss function as a constraint, after the neural network reaches a certain number of learning times in each step of the optimization process, the total gradient value obtained from the neural network is used as the sensitivity of a single optimization step, and the total loss constraint and the sensitivity are added into the MMA optimizer for optimization. Finally, the typical design examples in the field of shock absorption and buffering are studied[3]. The results show that after adding the honeycomb structural gene into the optimization, the optimized structure obtains the hole features of the honeycomb, there are dense holes in the internal solid material of the structure, and it is found that the energy absorption effect per unit volume of the structure integrated with biological features is significantly improved than that of the original structure.

Fracture, damage and failure mechanics of cementitious materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

3D MESOSCALE FRACTURE INVESTIGATION OF ULTRA HIGH PERFORMANCE CONCRETE CONSIDERING FIBRE ORIENTATION CHARACTERISTICS

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ABSTRACT

Ultra high performance fibre reinforced concrete (UHPFRC) is composed of fibres, mortar, fibre-mortar interfaces, and pores randomly distributed in space. The damage and fracture of ultra high performance fibre reinforced concrete (UHPFRC) is inherently dependent on fibre orientation and distribution [1]. This work first carried out uniaxial tensile tests of UHPC where the fibres were oriented by an external magnetic field [2]. The fibres were thus subjected to the electromagnetic force and underwent directional distribution, i.e. along the magnetic field direction. Three groups of fibre orientation were used: parallel to the tensile direction, perpendicular to the tensile direction, and no magnetic field applied. This resulted in three groups of specimens termed aligned-UHPC (AUHPC), perpendicular-UHPC (PUHPC), and UHPC, respectively. The effects of fibre orientation on cracking processes and stress-strain curves of UHPC under tension are studied using image analyses and digital image correlation techniques. Secondly, a 3D mesoscale finite element model was developed, in which cohesive elements were pre-inserted in the mortar to simulate the energy dissipation in the fracture process zone and the opening/closing of discrete cracks [3]. Different fibre orientation distribution in AUHPC, UHPC, and PUHPC was generated using a random algorithm. The fibre-mortar interaction was equivalently modelled through fibre constitutive laws, which were curve-fitted from the pullout force-slip relations extracted from single fibre pullout tests for various inclination angles. The proposed model was validated by single fibre pullout tests and direct tensile tests. The mesoscale influencing factors on complex multiple cracking and fibre bridging mechanisms were also quantified.

Keywords
ultra high performance concrete; fibre orientation; digital image correlation techniques; cohesive interface model; 3D fracture simulation at mesoscale

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Predictive digital twins
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PROOF-OF-CONCEPT DIGITAL TWIN OF AN INDOOR FOOTBRIDGE USING A PARAMETRIZED STOCHASTIC REDUCED-ORDER MODEL

Jenmy Zhang[*1], Akmal Bakar[1], Farhad Javid[1], Patrick Nadeau[1], Adrian Humphry[1], Mehran Ebrahimi[1], Adrian Butscher[1], Alex Tessier[1], Jesus Rodriguez[1], Marie-Jo Azzi[2] and Charbel Farhat[2]*

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ABSTRACT

Uncertainty in digital twins is inevitable due to modeling assumptions, inherent randomness in the loads, sensor noise etc. The uncertainty must be quantified to ensure reliable predictions, but many of the sources of uncertainty lack an obvious parametric form. The stochastic projection-based reduced-order model (SPROM) [1] is a non-parametric approach for reducing and quantifying uncertainty in the digital twin via probabilistic model learning from sensor data. This talk presents the steps required to train a load parametrized SPROM for predicting the dynamic response of an indoor footbridge with quantified uncertainty. The input to the digital twin is a set of "what-if" loading parameters, or live measurements of the 6 strain gauges on the bridge, from which the loads can be inferred. The output is a probabilistic prediction of the physical structure's response under the specified loads, including quantities and regions of interests that are not directly monitored with sensors. Since the SPROM is a model updated from strain data, it captures the response and the associated uncertainty of a “healthy” structure. Hence the SPROM provides a baseline against which future changes in the structure can be reliably quantified and diagnosed. This is a unique advantage compared to alternative approaches (e.g., Kalman Filter) which forecast the immediate future state of the system. The contribution of this work lies in: 1) training an SPROM for a physical structure under complicated loads, and 2) using live monitoring data collected while the structure is fully operating. A key challenge is that the live loads producing the strain measurements are entirely random and not known in advance. To this end, we first leverage cameras installed on the bridge to extract 200 "events" of a single person crossing the bridge over 3 days. Second, we use a parametrized projection-based ROM to infer the walking loads for each event, the details of which are presented in a separate talk submitted to this mini-symposium. Third, we use stochastic gradient descent to optimize the "randomness" of the SPROM such that we maximize the likelihood of observing the strain measurements. Our initial results demonstrate the viability of the approach, even with “gappy” sensor data due to partial corruptions by unexpected bursts of electromagnetic interference.

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Machine learning for design tasks and inverse problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

KNOWLEDGE EXTRACTION FROM TIME SERIES SENSOR DATA USING NEURAL NETWORK

Farhad Javid[1], Patrick Nadeau[1], Akmal Bakar[1], Mehran Ebrahimi[1], Adrian Humphry[1], Jesus Rodriguez[1], Jenmy Zhang[1], Adrian Butscher[1] and Alex Tessier[1]*

[1]Autodesk

ABSTRACT

Complex civil structures such as bridges, towers, and buildings, are frequently monitored with a network of sensors that collect extensive physical and environmental data. This data is crucial in assessing the structural health and state, and in evaluating both short and long-term behaviours. Improved interpretation of monitoring data can be achieved by coupling it with digital twins—virtual replicas of physical systems. Digital twins can serve as essential tools for facilitating maintenance and operational tasks for civil structures, including health monitoring, fault detection, and performance evaluation. To utilize sensor data effectively, relevant knowledge for each specific digital twin should be extracted from raw data using sensor fusion. Sensor fusion involves the intricate process of mixing, augmenting, and filtering data from traditionally disparate sensors to obtain a comprehensive view of a system's state. For example, the excitation of the first mode of vibration in a bridge under moving traffic loads can be derived from displacement or strain data obtained from at least two sensors installed at distinct locations along the bridge. Neural Networks have shown promise in extracting knowledge from various sources, including images, texts, and graphs, by discerning patterns and rules within a learning process. In this study, we leverage real-world sensor data and exploit neural network capabilities to introduce a model for knowledge extraction from sensor data installed on civil structures. Specifically, we adapt UNet[1]—a convolutional encoder-decoder model with residual connections—to detect and parameterize walking loads on a pedestrian bridge. The model utilizes strain gauge data from three locations along the bridge and distinctively identifies walking events by precisely determining their start (when the pedestrian enters the bridge) and end (when they leave) times. Next, an encoder convolutional model is trained on the data to ascertain walking load parameters such as speed, step frequency, and load magnitude. Our results show that neural networks, if carefully tuned and trained, can serve as versatile sensor fusion tools capable of identifying a structure's state with a minimum number of sensors, potentially reducing the cost and complexity of sensor systems on civil structures.

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Mini-symposium in memory of Professor J. Tinsley Oden honoring his lifetime achievements in computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

UNDERSTANDING NEURODEVELOPMENTAL DISORDERS USING ISOGEOMETRIC ANALYSIS, THB-SPLINES AND ADAPTIVE DOMAIN EXPANSION

Jessica Zhang[*1] and Kuanren Qian*[1]

[1]*Carnegie Mellon University*

ABSTRACT

In the US, neurodevelopmental disorders (NDDs) have emerged as the most prevailing chronic medical conditions in the pediatric population, with a notable increase from 6.3% in 1997 to 10.8% in 2021. Comprised of a diverse group of diseases such as autism spectrum disorder (ASD), attention deficit hyperactivity disorder (ADHD), and epilepsy, NDDs are characterized by substantial impairments to cognitive, speech, memory, motor, and other neurological functions, exerting life-long detrimental effects on patients. These symptoms arise due to disruptions of the neurodevelopmental process, leading to severe adverse impacts on the growth of neurons and the formation of vital central and peripheral nervous systems. However, the heterogeneous nature of NDDs presents formidable challenges in identifying the underlying etiology, facilitating accurate diagnosis, and administering the necessary treatments. A competent computational neuron growth model holds immense potential to advance our understanding of multifaceted factors behind the growth process, contribute to the development of potential treatments, and identify the underlying root causes. In this study, we introduce a novel 3D neuron growth model utilizing the phase field method and isogeometric analysis (IGA) to model intricate neurite outgrowth. Leveraging adaptive domain expansion, our model can efficiently expand the domain as needed based on neurite outgrowths to lower computational costs by minimizing the degrees of freedom. With truncated hierarchical B-splines (THB-splines), our model can adeptly simulate complex neurite structures on coarse mesh while preserving accuracy by applying multiple levels of local refinements. Extending beyond the computational model, we conduct comprehensive investigations of neurodevelopmental disorders using the computational model to unveil the effect various factors have on the growth process.

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Industrial applications of IGA
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HYBRIDOCTREE_HEX: HYBRID OCTREE-BASED ADAPTIVE ALL-HEXAHEDRAL MESH GENERATION WITH JACOBIAN CONTROL

Jessica Zhang[*1] and Hua Tong*[1]

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ABSTRACT

We present a new software package, “HybridOctree Hex,” for adaptive all-hexahedral mesh generation based on hybrid octree and quality improvement with Jacobian control. The proposed HybridOctree Hex begins by detecting curvatures and narrow regions of the input boundary to identify key surface features and initialize an octree structure. Subsequently, a strongly balanced octree is constructed using the balancing and pairing rules. Inspired by our earlier preliminary hybrid octree-based work, templates are designed to guarantee an all-hexahedral dual mesh generation directly from the strongly balanced octree. With these pre-defined templates, the sophisticated hybrid octree construction step is skipped to achieve an efficient implementation. After that, elements outside and around the boundary are removed to create a core mesh. The boundary points of the core mesh are connected to their corresponding closest points on the surface to fill the buffer zone and build the final mesh. Coupled with smart Laplacian smoothing, HybridOctree Hex takes advantage of a delicate optimization-based quality improvement method considering geometric fitting, Jacobian and scaled Jacobian, to achieve a minimum scaled Jacobian that is higher than 0.5. We empirically verify the robustness and efficiency of our method by running the HybridOctree Hex software on dozens of complex 3D models without any manual intervention or parameter adjustment. We provide the HybridOctree Hex source code, along with comprehensive results encompassing the input and output files and statistical data in the following repository: https://github.com/CMU-CBML/HybridOctree_Hex.

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Recent advances on interfaces dynamics modeling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ROTATION-INDUCED TRAUMATIC BRAIN INJURY: A FLUID MECHANICAL STUDY

Jiaqi Zhang[1], Qifu Wang[2], David Bates[2], James Feng[3], Pengtao Yue[4] and Qianhong Wu[2]*

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ABSTRACT

Traumatic brain injury (TBI) is a significant health concern, with rotation-induced TBI being particularly severe. To gain a deeper understanding of this issue, we have developed a finite-element code to simulate the impact dynamics in a simplified setup. The model involves a spherical hydrogel ball, representing the soft brain matter, suspended in a fluid within a transparent cylinder. The hydrogel ball is treated as a poroelastic material infused with fluid, and its interaction with the surrounding fluid is managed using an arbitrary Lagrangian-Eulerian method. Our simulations reveal that the contrast in density between the ball and the fluid, as well as the difference in rotational velocity, are key factors in the deformation of the ball due to centrifugal forces.

To validate and further explore these findings, we conducted experiments where the hydrogel ball was subjected to controlled rotation within a water bath, which emulates the cerebrospinal fluid (CSF). Measurements of the cylinder and ball velocities, along with the deformation of the ball over time, were taken. Our experimental results corroborate the computational findings, showing that phases of acceleration and deceleration are most likely to cause damage to the brain model.

This combined numerical and experimental approach provides valuable insights into the role of CSF in transmitting impact from the skull to the brain, contributing to our understanding of brain injuries. It may also portend the development of preventive measures and improved treatment strategies.

AN OPTIMAL IMPLICIT SINGLE-STEP SINGLE PARAMETER TIME INTEGRATION METHOD FOR STRUCTURAL DYNAMICS

Jie Zhang[1]*

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ABSTRACT

A comprehensive study of the implicit second-order-type time integration methods for structural dynamics analysis is presented. An analytical accuracy framework for algorithm design, convergence, and optimization is developed, where the obstacles encountered in algorithms design, convergence accuracy, algorithms equivalence, accuracy measurement, and accuracy optimization in traditional accuracy frameworks are addressed. An Optimal linear multistep method Equivalent Single-step method with a Single parameter (OESS) is revealed, where the controllable parameter can provide desirable performance on the low-frequency accuracy and high-frequency numerical dissipation properties. The OESS methods is second-order accurate, unconditionally stable, overshooting acceptable, and equivalent to an optimal route between the Houbolt method and the trapezoidal rule.

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Catastrophic failure mechanics and numerical modelling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ON IRRADIATION-INDUCED MULTI-SCALE DEFORMATION BEHAVIORS OF ACCIDENT TOLERANCE MULTI-LEVEL COMPOSITE FUELS

Jing Zhang[*1] and Shurong Ding[1]*

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ABSTRACT

FCM(Fully Ceramic Microencapsulated) fuel pellet is a potential accident tolerance multi-level composite nuclear fuel, which consists of dispersed TRISO(Tri-structural Isotropic) fuel particles embedded within the SiC matrix. TRISO fuel particle in the FCM fuel has a multi-layered structure, and the innermost fuel layer called Kernel is coated by four functional layers, namely the porous pyrolytic carbon (Buffer) layer, the inner dense pyrolytic carbon (IPyC) layer, the silicon carbide (SiC) layer, and the outer dense pyrolytic carbon (OPyC) layer. Owing to the excellent fission product retention capacity of TRISO particles and the strong stability of the SiC matrix, FCM fuel pellet is suitable for many advanced nuclear reactors and is an important development direction of advanced fuel. In order to perform the manufacturing and optimal design of FCM fuel as well as ensure its safety and cost-effectiveness for practical use in reactors, it's necessary to study the irradiation-induced thermal-mechanical coupling behaviors of FCM fuel.
FCM fuel exhibits more complex irradiation-induced thermal-mechanical coupling behaviors than conventional nuclear fuel owing to its multi-level composite structure. Kernel can produce complicated fission gas-thermal-mechanical coupling behavior. The porous Buffer layer also undergoes multi-scale thermal-mechanical coupling behavior due to the interaction of multiple physicochemical processes. The IPyC layer and OPyC layer have anisotropic irradiation deformations. The irradiation swelling and creep deformation occur within the SiC layer and matrix under irradiation conditions. Meanwhile, thermal-mechanical interactions also appear between each layer, as well as between TRISO particles and matrix. It can be concluded that FCM fuel produces complex multi-scale thermal-mechanical coupling behaviors.
In this study, the irradiation effects of each part of the material are comprehensively considered, and then the multi-scale correlating irradiation-induced thermal-mechanical constitutive models, calculation methods and subroutines are developed. The numerical simulation of multi-scale deformation behaviors of FCM fuel is performed more accurately. Based on the obtained evolution rules, the safety of FCM fuel during reactor service is analyzed. The influence of particle coating layer thickness on the multi-scale deformation behaviors in FCM fuel is also investigated, and the optimization of structural design parameters is proposed in view of ensuring economy and safety. This study can put forward a theoretical basis and technical support for the optimal design and advanced manufacturing of FCM fuel pellets.

Modeling and simulation of dynamics, stability and control of aerospace structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RESEARCH ON THE ANALYSIS OF MOTION STATE IN ORBIT AND ORBIT KEEPING CONTROL OF TETHERED SATELLITE SYSTEM

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ABSTRACT

Tethered Satellite Systems (TSS) have significant research and application value in areas such as artificial gravity, space elevators, gravity stabilization, orbit transfer, and tether formation flying. Due to the unique spatial structure of TSS, its dynamic behavior exhibits high nonlinearity. This paper investigates the on-orbit dynamics and orbit control problem during the state maintenance phase of a two-body TSS. Firstly, the TSS is modeled as a "double mass point with a mass elastic rod" system, and the general form of the dynamic equations for the five degrees of freedom is established based on Lagrange's equations. Taking into account the J2 perturbation, the dynamic equations for the five degrees of freedom under the influence of Earth's oblateness are derived. Next, the geostationary satellite orbit is taken as the reference baseline for the system's center of mass orbit, and the effects of the J2 perturbation on both the five-degree-of-freedom and three-degree-of-freedom TSS are analyzed using numerical methods. The results show that the J2 perturbation causes periodic variations in the height of the system's center of mass, with a maximum deviation of approximately 1 km. However, its impact on the system's true anomaly, in-plane and out-of-plane attitude angles, and tether length is minimal, although it follows certain patterns. Finally, two classical PID control methods are selected to primarily maintain control over the height of the center of mass in the three-degree-of-freedom system. Control rates are proposed, and the results demonstrate that the position-based PID controller can compensate for the influence error of the J2 perturbation on the system's center of mass orbit. However, its control performance in terms of maximum deviation and oscillation is average. On the other hand, the incremental PID controller can achieve the desired orbit maintenance effect. It exhibits smaller maximum deviation, shorter control adjustment time, and fewer oscillations compared to the position-based PID controller, resulting in significant improvements in control performance indicators. In conclusion, this study provides valuable insights for the research on orbit control of nonlinear Tethered Satellite Systems.

Recent advances on interfaces dynamics modeling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A FINITE-DIFFERENCE APPROACH FOR MEMBRANE VISCOSITY IN CAPSULE DYNAMICS SIMULATIONS

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ABSTRACT

The dynamics motion, deformation and interaction of biological and artificial capsules in flows, as well as the suspension rheology, are of great interest for biomedical research and applications. When undergoing a strain change, viscous stress is resulted in the capsule membrane, and such viscous behaviors have been noticed decades ago. To model the membrane viscosity, several numerical methods had been developed; however, serious concerns are noticed in these methods, such as physical misrepresentation, mathematical inconsistency and numerical complexity. In this presentation, a simple and efficient algorithm is proposed for calculating the membrane viscous stress for simulating capsule dynamics in fluid flows. The method was developed by applying finite-difference approximations, and rigorous validations have been performed to demonstrate its accuracy, efficiency and stability. This method has been employed in several studies of red blood cell behaviors in various flow situations. Application examples will also be presented.

Advances and applications of polytopal methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN IMPLICIT-EXPLICIT TIME INTEGRATION FOR DAM-FOUNDATION INTERACTION BASED ON OCTREE MESH USING SCALED BOUNDARY FINITE ELEMENT METHOD

Junqi Zhang[*1], Pengcheng Liu[1], Mi Zhao[1] and Xiuli Du[1]*

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ABSTRACT

In this study, we propose a novel implicit-explicit time integration scheme for dynamic analysis of dam-foundation interaction. In engineering practice, it is necessary to model the dam using a refined mesh with elements smaller than a meter in size, while the foundation, encompassing the larger geological region and underlying soil, is typically represented with a mesh using elements of ten meters or greater. This nonuniform mesh usually leads to difficulties in numerical modeling and analysis. In explicit time integration, the critical stable time step is governed by the smallest elements in the dam, while the implicit scheme consumes excessive memory and computational power. To address these challenges, we propose a hybrid time integration scheme, in which the dam's dynamic behavior is calculated using the implicit method, while the surrounding foundation is calculated using the explicit method with a larger time step. A specially designed overlapping layer is devised to facilitate data communication between the implicit and explicit regions. To this end, we employ the octree algorithm to generate the mesh automatically, exploiting its distinct advantages in rapid mesh size transition and high element quality. The polyhedral elements in the octree mesh are formulated using the scaled boundary finite element method, without necessitating any special treatment. Numerical examples are presented to demonstrate the efficiency and effectiveness of the proposed method.

Modeling and simulation of the electro-chemo-thermo-mechanical interactions in energy transition and energy storage systems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHASE FIELD MODELLING OF ELECTROCHEMICALLY DRIVEN VOID EXPANSION AND SPONGE FORMATION IN SILICON ELECTRODES OF LITHIUM-ION BATTERIES

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ABSTRACT

Recent experimental studies have shown that the silicon electrodes of lithium-ion batteries undergo microvoid expansion and merging during electrochemical cycling, forming sponge-like internal channels, which then penetrate the original surface of the silicon material and further form new surfaces. This microstructural change leads to irreversible deformation of the silicon electrode, which has a significant negative impact on the mechanical integrity and cyclic stability of the cell.
In order to understand this unexpected microstructural evolution, we develop a theoretical model of mechanical-electrochemical coupling based on the phase field method to predict the annihilation, expansion, merging, and surface instability of microvoids. The electrochemical cycle simulation reveals the following microstructure evolution mechanism and images: the surface pits continue to expand on the surface, the internal microvoids expand and move towards the surface of the electrode material, and the microvoids expand in the direction of mutual proximity, resulting in the merge of the voids, the formation of internal channels, and the penetration of the surface. Further, we found that this undesirable spongy microstructure, which is detrimental to battery performance, can be suppressed by mechanical stress.

Multiscale modeling, analysis and numerical methods of material defect and inhomogeneities
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

LIFTING TO HIGHER DIMENSIONS — ALTERNATIVE WAY FOR MULTISCALE COMPUTING

Lei Zhang[*1]*

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ABSTRACT

Most multiscale computing techniques are based on dimension reduction. In this talk, I will present an alternative approach for multiscale computing by lifting problems into higher dimensions. Through a few examples, including periodic/quasiperiodic homogenization, quantum algorithms for multiscale PDEs, etc., I will demonstrate how lifting into higher dimensional spaces can enable accurate and efficient multiscale modeling and simulation.

Machine learning and multiscale modeling for complex materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL INVESTIGATION ON THE MODULATION OF WRINKLING IN TENSEGRITY-MEMBRANE STRUCTURES

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ABSTRACT

Tensegrity-membrane structures are potential to be lightweight gossamer spacecraft (e.g., solar sails, radar antennae, solar module), and the dynamics of deployment has been studied in the past studies where the membranes were usually modeled as a flat panel without wrinkles. However, the attitude control of membrane as well as the flatness are critical to the functionality of gossamer spacecraft. The paper proposes a numerical investigation on the modulation of wrinkling in tensegrity-membrane structures. The kinematic and deformation description are based on the co-rotational finite element method (FEM), while the wrinkling of membrane is modeled by Tension Filed Theory (TFT). The numerical method is validated by an illustrative experiment, and then used for a surrogate model-based optimization design, in which clustered actuation is responsible for the attitude control of membrane, while classical actuation accounts for the suppression of wrinkles. An interesting tensegrity-membrane "Sunflower" is presented to show the result of optimization, where "Sunflower" can follow the sunlight Angle accurately and freely control the orientation of "corolla" while maintaining its daylighting surface quality. This study provides effective means for the numerical simulation and optimization design of tensegrity-membrane structures, especially when the attitude and wrinkling of membranes must be considered.

Keywords: tensegrity-membrane structure; the co-rotational FEM; wrinkling model; surrogate model-based optimization; classical and clustered actuation

Causal discovery and graphical causal models
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CAUSALNO: DISCOVERING HIDDEN CAUSAL MECHANISMS FROM MECHANICAL TESTING DATA.

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ABSTRACT

Deep neural networks, such as neural operators, have emerged as powerful tools for learning and predicting the response of a complex physical system solely from observational data. This is evident in material modeling problems, where the neural operator approach learns a surrogate mapping from the loading field to the corresponding material response field. It can be seen as learning the solution operator of a hidden Partial Differential Equation (PDE), where the microstructure and mechanical parameters of material specimens correspond to the (potentially heterogeneous) parameter field within this PDE. Consequently, the predictive material modeling problem becomes akin to a forward problem for PDEs.

However, amidst this progress, the discovery of hidden physical properties and the physical interpretation of these data-driven material models remain less explored. To address this gap, we propose to discover the latent representation and causal relationships behind neural operators, effectively solving an inverse problem for PDEs. In particular, we introduce a novel hyper neural operator architecture to learn and extract latent representations from neural network parameters. To enhance the interpretability of these latent representations, we incorporate a Structural Causal Model (SCM) that captures the underlying causal mechanism governing the hidden physical process. Experiments show that CausalNO, our proposed approach, can effectively learn interpretable and generalizable representations from both simulated and real mechanical testing data.

Numerical methods, mathematical modeling and analysis in material science
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STRUCTURES AND DYNAMICS OF HETERO-INTERFACES BASED ON UNDERLYING MICROSTRUCTURE

Luchan Zhang[*1]*

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ABSTRACT

The hetero-interfaces are commonly formed between different materials or different phases to accommodate the lattice misfit between the adjacent materials.
The structure and dynamics of hetero-interfaces strongly affect the mechanical, electronic and plasticity properties of the composite materials and alloys. The structure of a hetero-interface is a network of dislocations and disconnections, together with the inclination and misorientation of the interface. The motion of the hetero-interface, such as the precipitation inα/βtitanium alloys and martensitic transformations, is also controlled by the interface network structure of disconnections. We present continuum models for the structure and dynamics of hetero-interfaces based on the continuum distribution of these line defects on them.

The phase field method for fracture: Theory, numerics, and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPLORING MULTI-PHYSICAL COUPLED FRACTURE IN POLYMERS THROUGH PHASE-FIELD MODELING

Lu-Wen Zhang[*1]*

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ABSTRACT

Polymers have emerged as key materials for achieving structural-functional integration in marine engineering owing to their remarkable properties such as chemical corrosion resistance, damping characteristics, high specific strength and fatigue resistance. However, prolonged exposure of these materials to the marine environment exposes them to a variety of complex environmental and mechanical loads, resulting in nonlinear, multi-process coupled fracture phenomena. In response to this challenge, we have developed phase field models and efficient finite element programs to systematically investigate the thermodynamic processes associated with moisture diffusion-thermo-mechanical coupled fracture in polymers and composites in high-moisture environments. Our research focuses on the transient two-way coupling behavior between moisture diffusion and crack propagation in composites, providing a comprehensive understanding of the intricate interactions. The investigation of the moisture absorption-induced damage mechanism offers in-depth insights into the degradation process. Our methodology demonstrates its capability to accurately track experimentally consistent crack nucleation and propagation, regarding a wide range of strain rates and cyclic impact loading conditions.

Machine learning and multiscale modeling for complex materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CHARACTERIZING STEEL CORROSION IN CONCRETE USING X-RAY COMPUTED TOMOGRAPHY AND MACHINE LEARNING TECHNIQUES

Mingyang Zhang[1] and Weilun Wang*[1]

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ABSTRACT

The corrosion of steel in concrete has been regarded as one of the most predominant factors for the degradation of reinforced concrete (RC) structures. The accurate predictions of corrosion damages are the basis for the safety assessment of in-service structures and the enhancement of new structure designs. X-ray computed tomography (XCT), known for its non-destructive capabilities, has been widely utilized to understand the corrosion process inside the concrete, offering three-dimensional (3D) visualization and aiding in the identification of steel corrosion [1]. This study uses U-Net, a deep learning network, to detect various phases of steel corrosion evolution in concrete, including the identification of rebar, corrosion products, pores, cement mortar, and corrosion-induced cracking. A galvanostatic accelerated corrosion test was performed to simulate rebar corrosion within the concrete. The XCT test was performed, producing a series of XCT images that reveal the corrosion-induced cracks in the concrete. This set of images formed a comprehensive training database for the U-Net model. The performance of the model was significantly improved by data augmentation within the training dataset, thereby enabling it to recognize corrosion-induced cracking and pores. The U-Net model proved effective in accurately segmenting the XCT images into different phases, demonstrating high accuracy on the test dataset. This significant advancement has automated the process of visualizing and 3D reconstructing the steel corrosion process inside the concrete.

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Computational models and methods for predicting cancer progression and treatment response
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PERSONALIZED PREDICTIONS OF GLIOBLASTOMA INFILTRATION: MATHEMATICAL MODELS, PHYSICS-INFORMED NEURAL NETWORKS AND MULTIMODAL SCANS

Ray Zirui Zhang[*1], Ivan Ezhov[2], Michal Balcerak[3], Andy Zhu[4], Benedikt Wiestler[2], Bjoern Menze[3] and John Lowengrub[1]*

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ABSTRACT

Predicting the infiltration of Glioblastoma (GBM) from medical MRI scans is crucial for understanding tumor growth dynamics and designing personalized radiotherapy treatment plans. Mathematical models of GBM growth can complement the data in the prediction of spatial distributions of tumor cells. However, this requires estimating patient-specific parameters of the model from clinical data, which is a challenging inverse problem due to limited temporal data and the limited time between imaging and diagnosis. This work proposes a method that uses Physics-Informed Neural Networks (PINNs) to estimate patient-specific parameters of a reaction-diffusion PDE model of GBM growth from a single 3D structural MRI snapshot. PINNs embed both the data and the PDE into a loss function, thus integrating theory and data. Key innovations include the identification and estimation of characteristic non-dimensional parameters, a pre-training step that utilizes the non-dimensional parameters and a fine-tuning step to determine the patient specific parameters. Additionally, the diffuse domain method is employed to handle the complex brain geometry within the PINN framework. Our method is validated both on synthetic and patient datasets, and shows promise for real-time parametric inference in the clinical setting for personalized GBM treatment.

STOCHASTIC SUBSPACE VIA PROBABILISTIC PCA FOR CHARACTERIZING AND CORRECTING MODEL ERROR

Akash Yadav[1] *and Ruda Zhang**[1]

[1]*University of Houston*

ABSTRACT

Complex engineering systems give rise to high-dimensional computational models that resolve multi-physics coupling and multi-scale processes, pushing the ever-expanding limit of computing power. Yet errors in system input, model parameters and model representation limit the predictive value of such models. Such model error shall be quantified and adjusted based on experimental measurement data, for predictive modeling and digital twinning. A seminal work [1] on this topic proposed a stochastic surrogate model that consists of projection-based reduced-order models (ROM) derived from a high-dimensional model, where the reduced-order bases are randomized. The use of ROM allows tractable uncertainty quantification, while learning a probabilistic model for the basis can improve model accuracy. We follow this strategy and design new probabilistic models for stochastic ROM.

Specifically, we propose a probabilistic model of subspaces based on the probabilistic principal component analysis (PCA). Given a sample of system state vectors, commonly known as a snapshot matrix, this method uses quantities derived from the PCA to construct distributions of the sample matrix as well as subspaces of all dimensions of the state space. It is applicable to projection-based reduced-order modeling methods, such as proper orthogonal decomposition and related model reduction methods. The stochastic subspace thus constructed can be used, for example, to characterize model error in computational mechanics. With experimental validation data, the stochastic subspace model can be adapted in a Bayesian approach to correct model error and improve accuracy.

The proposed method has multiple desirable properties:
(1) it is naturally justified by a probabilistic interpretation of PCA, and in some cases has analytical forms for the induced probabilistic models on related matrix manifolds;
(2) it satisfies linear constraints, such as boundary conditions of all kinds, by default;
(3) it has only one hyper-parameter, which dramatically simplifies the training procedure;
(4) its algorithm is very easy to implement.
We compare the proposed method with existing approaches [1,2] visually in a low-dimensional example, and demonstrate its performance in modeling the dynamics of a space structure.

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Uncertainty quantification and reliability analysis in engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

POLYNOMIAL CHAOS REPRESENTATION OF NON-GAUSSIAN RANDOM FIELDS BASED ON THE OPTIMAL TRANSPORTATION

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ABSTRACT

In this paper, we develop a methodology for constructing polynomial chaos (PC) representation of non-Gaussian non-stationary random field by optimal transportation theory. Firstly, non-Gaussian field samples, which is generated by the simulation technique proposed by current author, are represented by the truncated Karhunen-Loeve (KL) expansion. Then, the transformation from standard Gaussian variables to KL coefficients is directly constructed from the samples of KL coefficients by using optimal transportation. With the transformation from Gaussian to KL coefficients, the Hermite PC coefficients are further determined by using least square regression. Since the optimal transportation enables to move the source measure to target measure without requiring the absolute continuity of the target, the transformation from standard Gaussian to KL coefficients can be readily constructed from samples of KL coefficients, by passing the curse of dimensionality encountered in constructing PC representation by Rosenblatt transformation. Moreover, the current work generalizes the PC representation of random fields from translation-based one to more general non-Gaussian cases. Three numerical examples demonstrate the application of the developed method.

Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEM STUDY ON EVOLUTION OF SOIL ARCHING IN GROUND WITH TUNNEL

Ruixiao Zhang[*1], Dong Su[1], Xingtao Lin[1] and Xiangsheng Chen[1]*

[1]*Shenzhen University*

ABSTRACT

The effects of existing tunnels on the evolution of soil arching require further investigation. In this study, trapdoor models with different distances between the trapdoor and tunnel are examined via discrete element method simulations after a numerical model is established based on experiments. The results show that as the distance between the tunnel and trapdoor (L) increases, the minimum soil arching ratio, ultimate soil arching ratio, and load recovery decrease, thus indicating that the shadowing effect of the tunnel becomes less distinctive. The stress ratio in the region near trapdoor first decreased significantly and then gradually, followed by a gradual decrease as the trapdoor displacement increased, before reached an ultimate value. The reverse trend is observed when L exceeds 150 mm, which is similarly observed in regions L2 and L3. The displacement of particles above the tunnels was confined because of the shadowing effect caused by the tunnel, where the displacement was much lower than the displacement on both sides and above the weakly affected zone, and the particle displacement resulted in a flow around the tunnel. Two distinct types of soil-arching structures are identified for interaction and independent arches. The displacement of the trapdoor increased the anisotropy of the contact forces within the soil mass.

Advances in multi-scale, multi-material, and multi-component Topology Optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NON-PARAMETRIC GEOMETRY PATCHING TECHNIQUE FOR MMC TOPOLOGY OPTIMIZATION

Shengqi Zhang[*1], Weisheng Zhang[1], Sung-Kie Youn[2] and Xu Guo[1]*

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ABSTRACT

MMC is one of the topology optimization methods that provides explicit boundary description of the optimized topology. However, due to the inherent nature of MMC, the obtained geometry could exhibit distinct local singularities. To cope with this issue, a non-parametric geometry patching technique for MMC is developed. A moving-node patching technique for both two-dimensional and three-dimensional cases is developed in conjunction with MMC to obtain structures with smooth boundaries. Numerical examples in two-dimensional and three-dimensional are presented to demonstrate the effectiveness of the proposed approach.

Smart structures – Modelling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL ANALYSIS OF FUNCTIONALLY GRADED MAGNETO-ELECTRO-ELASTIC PLATES AND SHELLS

Shun-Qi Zhang[1]*

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ABSTRACT

Magneto-electro-elastic (MEE) materials combine properties of magnetostrictive and piezoelectric effects, which can realize positive or reverse magnetoelectric conversion effectively. As a new type of advanced functional composite material, its appearance has set off a wave of MEE materials research. MEE materials have higher electromagnetic coupling performance than pure piezoelectric or piezomagnetic composites. The modelling and simulation techniques for such multi-physics coupled problems are still of great challenge. This paper intends to develop a finite element (FE) model coupled with magneto-electro-elastic fields for static and dynamic analysis of FG-MEE plates and shells. The FE model is derived by using the first-order shear deformation hypothesis with consideration of linear multi-physics coupled constitutive equations. Eight-node quadrilateral plate/shell elements are proposed for FG-MEE structures, including five mechanical DOFs at each node, one electric and magnetic DOF at each MEE layer of elements. The model is first validated by MEE laminated plates and shells, later applied to parametric study of FG-MEE structures with functionally graded electric and magnetic properties.

NATURE-INSPIRED GENERATIVE DESIGN RULES FOR ADDITIVE MANUFACTURING

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ABSTRACT

This work presents a nature-inspired generative design methodology to support innovation-driven design for manufacturing. It allows designers to create unpredicted but valuable components that can be directly integrated by modern manufacturing methods such as additive manufacturing. In this approach, the design of components is redefined as a series of elemental design instructions and emergence mechanisms that react to the design environment to generate innovative designs. Inspired by plant intelligence in nature, a set of “Design Genes” and “Design Hormones” are proposed which influence “design growth and development” through analogues of biological mechanisms. The design grows and develops from the actions of the genes and hormones, which do not know anything about the emergent shape or form of the design, they simply respond to the engineering environment. The hormones are encoded with genes in a “Design Seed”, and different designs can emerge from the same seed in response to different environments based on their influence on the seed. A practical algorithm is then presented to implement the emergence of design from a simple seed. A range of examples are tested to demonstrate the effectiveness of the proposed approach. This work contributes foundational nature-inspired generative design theory and processes to promote innovative design integrated with manufacturing systems moving from Industry 4.0 to 5.0.

Advances in multi-scale, multi-material, and multi-component Topology Optimization
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MACHINE LEARNING POWERED SKETCH AIDED DESIGN VIA TOPOLOGY OPTIMIZATION

Weisheng Zhang[*1] and Xu Guo[1]*

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ABSTRACT

Structural topology optimization is an important design tool in the conceptual design phase of a product. However, the current topology optimization design is mostly driven strictly based on mathematical and mechanical models. Although the innovative design can be automated, it mostly lacks effective manual experience guidance. To improve the efficiency of computer-aided structural design models, this work proposes a sketch-guided topology optimization approach based on machine learning. Using neural network-based style transfer techniques, computer-digitized/hand-drawn sketches are explicitly incorporated into topology optimization in the form of constraint functions. The obtained optimization results not only satisfy the requirements of optimal mechanical properties, but also fully demonstrate the design intention and requirements of designers. Numerical examples show that the proposed approach can effectively compensate for the lack of manual experience guidance for topology optimization.

Advanced computational modelling of wood, wood-based products, bio-composites, and timber structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A FAST CALCULATION METHOD FOR PREDICTING STEADY STATE ABLATIVE MORPHOLOGY OF C/C COMPOSITES

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ABSTRACT

Gasification-type ablative composites, typical ablative thermal protection materials, convert the absorbed heat into an outward mass flux through physical or chemical processes during ablation, which cause surface recession and the formation of steady surface morphology of the materials. The variations lead to the structural change and surface roughness increase, which affect the flight trajectory and attitude-control characteristics of the aircraft and even aggravates the aerodynamic heating behavior. Therefore, predicting the surface morphology of materials during steady-state ablation is important.

When designing ablative materials, a huge number of calculations are required for analyzing surface morphology. To effectively design these materials and reduce experiments, a fast effective and simple calculation method is required. Up to date, most of the computational methods for predicting ablative morphology are complex and time-consuming. A quick and effective prediction of the ablation morphology remains a challenge. We discovered an angular relationship between the local ablation velocity at each point of the material and the global ablation velocity. Then, a fast, effective, and simple numerical calculation method for steady-state ablation is proposed.

When taking the carbon/carbon composite as example, we show that the predicted morphology is consistent with the experimental observation. The calculation time- consuming is significantly reduced. In addition, our method is found to be useful for analyzing the physical and chemical properties and surface roughness of the material. This calculation method is suitable for the prediction of the steady state ablative morphology of gasification-type ablative composites with arbitrary cross-section shapes. Furthermore, it can improve the understanding of the interaction between composites and their surrounding environments and provides a guidance for the structural design of gasification-type ablative thermal protection materials.

Keywords: steady-state ablation; surface morphology; calculation method; geometric characteristics

Multiphase flow and non-Newtonian fluid - Modelling and applications
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VISCOUS AND CAPILLARY EFFECTS IN THE SHOCK INDUCED BREAKUP OF CYLINDRICAL DROPLET: A NUMERICAL STUDY

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ABSTRACT

The high-speed aero breakup of a liquid droplet extensively exists in engineering applications and academic researches, such as dissemination of bulk liquid medium, and secondary atomization in turbomachinery. In addition, the fuel droplets are directly shattered by the standing shocks in the scramjet engine. In above scenarios, the essential flow features can be modeled as shock induced droplet breakup (SIDB).

In the previous studies [1], five different breakup regimes are recognized based on Weber number We=(ρ_g u_g^2 d_0)⁄σ. With the increase of the We, various regimes are respectively vibrational, bag, bag-and-stamen, stripping, and catastrophic. Later, the breakup mechanism is regrouped into two regimes [2], namely Rayleigh-Taylor piercing (RTP) and shear-induced entrainment (SIE). Meanwhile, influence of the viscosity is further considered through Ohnesorge number Oh=μ_l⁄sqrt(ρ_l d_0 σ). Although lots of experimental and theoretical works have been done on this problem, a deeper understanding of the droplet breakup, especially the droplet size distribution in the later stage, is still necessary. On the other hand, due to the difficulties on algorithm, numerical simulations of SIDB considering both surface tension and viscous effects are seldom carried out.

In this work, by employing the recently developed tangent of hyperbola for interface capturing (THINC) method [3], we conduct a systematically numerical study on the two-dimensional SIDB. The shock Mach number is fixed to Ms=1.47, while the Weber number and Ohnesorge number are altered, in order to investigate the capillary and viscous effects on the droplet breakup process. Specifically, We ranges from 10 to 103, and Oh ranges from 10-2 to 102.

In addition to the droplet morphology and unsteady drag properties, we also focus on the droplet size distribution after the disintegration. The droplet size distribution is characterized by using the spatial Fourier transform of volume fraction field as
α̂(k)=∫α(x) e^(-ikx) dx
With the obtained volume fraction spectrum, we attempt to analyze the characteristics of the droplet size distribution for the typical breakup regimes, and unravel how the surface tension and viscosity influence the final state of the shattered droplet.

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Constitutive modeling of complex materials with machine learning and artificial intelligence
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MODELING THE EFFECTS OF FRACTIONAL VISCOELASTICITY IN CARDIOVASCULAR SOFT TISSUES

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ABSTRACT

While experimental evidence indicates that all cardiovascular soft tissues exhibit some degree of viscoelasticity, the effects of viscoelasticity on the functional properties of soft tissues are not well understood. Most computational models for cardiovascular soft tissue ignore viscoelasticity and assume hyperelasticity. This is due to challenges associated with developing viscoelastic constitutive models and the computational expense associated with viscoelastic simulations, which grows O(N^2) in time and O(N) in memory for storing the strain history. More recently, fractional viscoelasticity has increased in popularity and has been shown to successfully model a number of soft tissues.

We have developed a computationally efficient fractional viscoelastic framework with a similar computational cost to conventional hyperelastic models and demonstrated its efficacy in several applications. This includes a viscoelastic model for the human myocardium, where we examined its physiological implication in a computational model of an idealized left ventricle and circulatory system [1]. The importance of viscoelasticity during passive filling was demonstrated by examining ventricular motion and regional fiber strain and stresses [2]. We also introduced a new viscoelastic constitutive model for the human femoropopliteal artery (FPA) grounded in its microstructure. We analyzed the contributions of each intramural component to the overall viscoelastic response, where the viscoelasticity of the passive smooth muscle cells (SMCs) was twice that of the collagen fibers [3]. We further extended this model to evaluate the effects of aging between thoracic aortas (TA) and FPA in 18 subjects between 13 and 73 years old. The results matched well with the structural density measured from bidirectional histology. The results further show that the viscoelasticity of the SMCs in the FPA was twice that of the TA but remained stable with age, like those of the collagen. Fractional viscoelastic modeling is a valuable tool for studying the mechanophysiology of biological soft tissues and investigating the effects of pathological factors and aging. This will improve the fidelity of computational simulations investigating device-tissue interactions and contribute to improving their physical accuracy.

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Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PROGRAMMING THERMO-ACTIVE METAMATERIALS WITH TEMPERATURE-SENSING ADAPTIVE RESPONSES

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ABSTRACT

Plants can change their morphology upon environmental variations such as temperature. We envision programmable matters that can alter their physical properties in desirable manners based on user input or autonomous sensing. This vision motivates the pursuit of mechanical metamaterials that interact with the environment in a programmable fashion. Here, we use multi-physics topology optimization and hybrid fabrication to systematically create soft metamaterials with arbitrarily programmable temperature-switchable morphing shapes and nonlinear mechanical responses under large deformations. We explore both temperature-sensing passive [1] and active [2] materials, such as liquid crystal elastomers. We demonstrate that the programmed metamaterials can accurately morph into a wide range of complex target shapes and curvatures as well as realizing maximized spontaneous area expansion, precisely programmable area change, and temperature-switchable nonlinear force-displacement behaviors. The computational inverse design technique holds promise for a wide array of applications requiring function- and performance-driven design of active materials with freely tunable thermally adaptive behaviors.

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Fracture, damage and failure mechanics of cementitious materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

CONTINUOUS SIMULATION OF THE FIBRE-CRACK BRIDGING MECHANISM WITH IMPLICIT MODELLING OF THE FIBRE-MATRIX INTERFACE USING A PHASE-FIELD BEAM MODEL

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ABSTRACT

The fibre-crack bridging mechanism is a critical phenomenon in fibre-reinforced concrete, wherein the crack growth is hindered by the presence of fibres. The understanding of this mechanism is essential for the design and optimization of fibre-reinforced concrete. However, simulating the complex interactions between fibres and cracks remains a challenge due to the presence of multiple physical scales and interfaces involved.

In this study, we propose a phase-field beam model to integrate the fibre and the fibre-matrix cohesive-frictional interactions in single constitution. Fibre elements are fully coupled with the matrix mesh, assuming no relative movements between fibres and matrix, which reduces the model complexity and increases the simulation efficiency and robustness. Since the the relative movement between fibres and matrix is excluded, the beam elements cannot represent the exact position and deformation of the fibres. Therefore, in addition to the displacement field of the beam elements, the virtual strain phase-field and its gradient are introduced to regularize the position and deformation of real fibres. The energy dissipation functional due to fibre-matrix de-bonding and slipping, as well as the stored energy functional, are characterized by a fibre strain distribution function and the energetic degradation function, Key parameters calibrated according to fibre pullout test.
The proposed model is validated through simulations of multi-angle fibre pullout tests, direct tensile tests, splitting tests, and three-point bending tests of steel fibre reinforced concrete. The simulated results are well aligned with the experimental results in terms of load-displacement curves, crack patterns, and fibre stress-strain states. Compared to existing simulation approaches, such as direct methods that explicitly model fibres and interfaces, and indirect methods that embed fibres with equivalent stress-strain accounting for fibre-matrix debonding and slipping in the matrix, the proposed model exhibits advantages in computational efficiency and robustness (compared to direct methods) and mechanical interpretability (compared to indirect methods).

Multiphysics biomechanics of bio- and bio-inspired soft materials: Theory, simulation and experiments
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHYSICAL FIELDS LEADING STRUCTURE DESIGN STRATEGY FOR META-FIBER REINFORCED HYDROGEL COMPOSITES BY DEEP LEARNING

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ABSTRACT

Fiber-reinforced hydrogel composites are widely employed in many engineering applications, such as tissue engineering, drug release, and flexible electronics, with more flexible mechanical properties than continuous hydrogel materials. Comparing to the hydrogel strengthened by continuous fiber, the meta-fiber reinforced hydrogel provides stronger individualized design ability of deformation patterns and tunable stiffness, especially for the elaborate applications in joint, cartilage and organ. In this paper, a novel structure design strategy based on deep learning algorithm is proposed for hydrogel reinforced by meta-fiber to achieve a targeted mechanical property, such as stress and displacement fields. A solid mechanic model for the meta-fiber reinforced hydrogel is firstly developed to construct the dataset of fiber distribution and the corresponding mechanical properties of the composite. A deep learning algorithm, generative adversarial network (GAN), is then trained to characterize the relationship between the input data, namely stress or displacement field, and the output data, namely meta-fiber distribution. Based on the algorithm, the inverse design strategy is proposed to determine the meta-fiber distribution in the hydrogel composites, with targeted stress or displacement fields. The proposed GAN-based inverse structure design strategy is implemented to design meta-fiber reinforced hydrogel composite structure under specific operation conditions. The results show that the deep learning method may efficiently predict the structure of the hydrogel composite with satisfied confidence, under the premise of given stress or displacement field and has great potential for applications in drug delivery and flexible electronics.

HYPERELASTIC MATERIAL CRACK SIMULATION WITH PERIDYNAMICS UNDER COMPLICATED NEUMANN BOUNDARY CONDITION

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ABSTRACT

Hyperelastic materials are frequently observed in the natural world and engineering applications such as rubbers and animal soft tissues[1][2]. Modeling large deformation and progressive fracture of these materials under complicated loading condition is challenging for numerical simulation. In this work, we propose a novel ordinary state-based Peridynamics (PD) model to simulate the large deformation of hyperelastic material. To simulate the progressive fracture, we propose a critical stretch calculation method for hyperelastic material in peridynamics, which gives accurate relatives between the critical stretch and the surface energy release rate. A virtual stress field is proposed to apply the nonconforming Neumann boundary condition for peridynamics. Instead of applying the boundary force on boundary particles directly, we define a virtual stress field on the material body to implicitly apply the Neumann boundary condition. With the virtual stress, the complex boundary representation and tracking is avoided. Furthermore, to obtain better computational efficiency, we perform an efficient adaptive refinement by splitting a parent particle into several child particles directly which does not require any information from its adjacent particles. The state variables and neighbor list of the child particles can be obtained directly from their parent particles, so that the proposed adaptive refinement method is very efficient and can be easily applied in both 2D and 3D cases without complex adjacent particle list building. The numerical results show that the proposed method can simulate the crack growth in hyperelastic material under complicated Neumann boundary condition with great efficiency and accuracy.

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AN ENRICHED IMMERSED FINITE ELEMENT METHOD FOR THREE-DIMENSIONAL INTERFACE PROBLEMS

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ABSTRACT

Interface problems arise in many applications in science and engineering. Partial differential equations (PDEs) are often used to model interface problems. Solutions to these PDE interface problems often involve kinks, singularities, discontinuities, and other non-smooth behaviors, which often pose challenges in obtaining satisfactory solutions. The immersed finite element method (IFEM) is a class of numerical methods for solving PDE interface problems with unfitted meshes.

In this talk, I will present recent advances in the development and analysis of IFEM for solving 3D interface problems with general non-homogeneous jump conditions. The proposed method can be utilized on interface-unfitted tetrahedral and cuboidal meshes, even if the 3D interface surface has an arbitrary shape. Distinguished from many unfitted-mesh methods in the literature, our method follows the homogenization idea, and the enrichment functions are immediately determined by the jump data, which does not introduce any additional degrees of freedom to the system, but still leads to optimal convergence. The resulting homogenized IFE space is isomorphic to the standard finite element space on the same mesh, and the isomorphism is stable with respect to the interface location. This feature leads to the optimal h^2 conditioning independent of interface location, which allows us to build an efficient multigrid grid solver. Numerical examples will be provided not only to validate our theoretical results, but also to demonstrate the applicability of the method when dealing with some real-world 3D interface models.

A DOMAIN-INDEPENDENT INTERACTION ENERGY INTEGRAL IN NON-HOMOGENEOUS MATERIALS CONTAINING COMPLEX INTERFACES UNDER TRANSIENT THERMAL LOADING

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ABSTRACT

Nonhomogeneous materials have been widely used in aeronautics, astronautics, microelectronics, and medical fields. The complex service environments in those materials may affect material failure. Fracture failure is one of the typical failure modes during the service process of nonhomogeneous materials. The interaction energy integral method [1-3] is a direct method for solving fracture problems, which introduces a designable auxiliary field into the traditional J-integral. In this paper, a thermomechanical problem of a nonhomogeneous material with complex interfaces under transient thermal loading is solved using the domain-independent, interaction energy integral method. Combined with the Newmark integral method, the transient temperature field is analyzed first using the non-Fourier heat conduction model. Then the transient thermal fracture problem in the non-homogeneous material with complex interfaces is solved, and the mixed-mode, thermal stress intensity factors are obtained. It can be proved that the validity of the new integral is not affected by the material discontinuity at the interfaces. The overshooting phenomenon of transient temperature occurs in non-homogeneous materials based on the non-Fourier heat conduction theory, which must be considered in engineering applications of these materials under extreme thermal environments.

Keyword: Mixed-mode thermal stress intensity factors, thermal shock, interface

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Mesh-free particle methods for multi-physics problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

NUMERICAL INVESTIGATION ON HYDRODYNAMIC CHARACTERISTICS OF FLOATING OWC BREAKWATERS BASED ON MULTI-PHASE ASR-SPH METHOD

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ABSTRACT

The oscillating water column (OWC) breakwaters have superior performances in wave reduction and energy extraction, which has been proven nearly a decade ago. However, few scholars have used SPH method to investigate their pneumatic and hydrodynamic characteristics comprehensively, because the significant difference between aerodynamic scale near the chamber orifice and hydrodynamic scale of the wave tank leads to great particle numbers and unacceptable computational cost. In this work, GPU acceleration technique together with adaptive spacing resolution (ASR) is applied to multi-phase SPH method to simulate the floating OWC breakwaters. Three numerical cases, including wave interaction with box-type floating breakwaters, dam-breaking flow impacting on an elastic plate, and wave interaction with a fixed OWC structure, are simulated to validate the numerical models. Then, a floating OWC breakwater with the elastic plate is investigated by multi-phase ASR-SPH. A series of simulations are conducted under different wave conditions to discuss the performances of OWC devices and the dissipation characteristics of wave energy. Results show that the valley value of wave transmission coefficient and the peak value of wave energy extraction capability occur at the same relative width position, indicating that the wave energy extraction of the floating breakwater has a great effect on its wave protection performance. Also, as the length of the elastic plate increases, the shear behavior of water at the end of the elastic plate is significantly enhanced, leading to a significant increase in vortices.

Architected materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THE PERFORMANCE OF METALLIC HONEYCOMB STRUCTURES SUBJECTED TO HIGH TEMPERATURES

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ABSTRACT

Architected cellular materials exhibit exceptional mechanical properties, such as ultralight, ultrastiff, and even respond to external stimuli through tailoring geometry and topology rather than changing composition. Such materials have the potential to be applied in the aerospace industry, automotive and mechanical engineering, and energy sectors, which usually require them to perform under high-temperature environments. Despite this, limited research investigated the performance of architected cellular materials under high temperatures. To address this gap, our study utilizes recent advances in additive manufacturing to create a series of heat-resistant alloy honeycomb structures using ABD-900AM. This research focuses on the processing, characterization, and analysis of the deformation behavior of these metallic honeycomb structures at both room temperature and 900°C. Through a combination of experiments and simulations, we have gained a comprehensive understanding of the deformation mechanisms and their interaction with damage pathways across various temperatures. Additionally, we explored the effects of oxidation and the intrinsic ductility of the material.

THE RELATIONSHIP BETWEEN MICROSTRUCTURES AND MECHANICAL PROPERTIES IN ADDITIVE MANUFACTURING

Zhao Zhang[1], Yifei Wang[1], Lichao Zhang[1], Xiang Gao[1], Hongshan Zhou[1] and Jingyuan Chen[1]*

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ABSTRACT

The formation of microstructures determined by the high cooling rate is the key reason for the mechanical properties in additive manufacturing. The relationship between microstructures and mechanical properties is necessary to be established for the design of mechanical properties based on the control of the microstructural evolutions. Here Monte Carlo model and phase field model are used to determine the grain morphologies in additive manufacturing and a dislocation evolution model is integrated with the crystal plasticity model to calculate the mechanical properties of additively manufactured specimens. The relevance between the process parameters and the microstructures is studied and then the relationship between microstructures and mechanical properties is investigated. Experiments are carried out for the validation of the proposed model. The yield strength can be decreased in high temperatures, which is caused by the synergies of grain globularization and vacancy concentration in high temperature states.

Recent advances on interfaces dynamics modeling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A SECOND-ORDER HYBRID IIM-PFEM METHOD FOR TWO-DIMENSIONAL MOVING CONTACT LINE PROBLEMS

Zhen Zhang[*1]*

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ABSTRACT

We develop a second-order Cartesian grid based numerical method to solve two-dimensional moving contact line problems, which are modeled by the incompressible Navier-Stokes equations with the Navier-slip condition and the contact angle condition (CAC). The solutions of the flow field and the interface motion are decoupled in an alternating way. For a given interface, the velocity field is solved via a pressure Poisson equation formulation of the incompressible Navier-Stokes equations, which is numerically discretized by the immersed interface method. Once the velocity field is obtained, the interfacial kinematics together with the CAC is reformulated into a variational system, which is solved by the parametric finite element method (PFEM). With this hybrid method, we detect topological changes in the interface by the inconsistency of neighboring normal vectors, which are directly computed through the parametric FEM. Second-order accuracy of the proposed method in both the interface and the contact line positions before and after topological changes has been numerically validated. Moreover, with the help of the numerical method, the merging and collision dynamics of droplets on the substrates are easily investigated.

Accelerating failure predictions through advances in scientific machine learning and scientific computing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ADAPTIVE ALARM SYSTEM FOR PREDICTIVE MAINTENANCE OF ELECTRIC MOTORS

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ABSTRACT

Electric motors are widely used in various fields such as production lines, robots, ships, and electric vehicles. They are one of the most fundamental and critical actuators in the field of industrial automation. However, if mechanical faults in motors are not detected and addressed promptly, it can affect the performance and lifespan of the motors, leading to issues such as production equipment downtime, decreased product quality, and energy waste. Therefore, this paper presents an adaptive alarm system for predictive maintenance of motors based on machine learning.

The system autonomously collects vibration data from motors and utilizes the random forest algorithm and the WDCNN deep convolutional neural network model to establish a comprehensive predictive model for data analysis and processing. Through machine learning, the system predicts the fault type of new input data and promptly issues an alarm signal. The system employs the Adam optimization algorithm with adaptive learning rates to improve the accuracy and reliability of the model. The results of cross-validation and testing experiments demonstrate that the proposed adaptive alarm system can achieve predictive maintenance of motors, effectively enhancing their reliability and safety. The predictive model exhibits good robustness and generalization ability, enabling it to adapt to different types and degrees of mechanical faults.

Keywords: motor fault diagnosis, deep learning, adaptivity, alarm system, predictive maintenance.

Computational mechanics for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

COMBINING SYNCHROTRON X-RAY DIFFRACTION AND MECHANISTIC MODELING FOR STUDYING MELT POOL DYNAMICS DURING CERAMICS LPBF

Zhilang Zhang[1], Makowska Malgorzata Grazyna*[2], Mohamadreza Afrasiabi[3] and Markus Bambach[1]*

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ABSTRACT

Laser Powder Bed Fusion (LPBF), a 3D printing technology, can produce parts with complex geometries that are typically difficult to create using conventional manufacturing techniques. However, the complex phenomena related to the melting and solidification of powder particles pose significant challenges for both experimental and numerical tools in terms of investigating and, furthermore, controlling the print quality. In this work, the evolution of the melt pool in ceramics LPBF is observed at the Tomcat beamline of the Paul Scherrer Institute using operando high-speed tomographic microscopy. As a Lagrangian and particle-based discretization technique, the smoothed particle hydrodynamics (SPH) method [1] provides distinct advantages in handling large deformations and capturing moving interfaces encountered in LPBF simulations [2]. We present a particle-based SPH solver to simulate the LPBF process and test its validity by comparing the simulation results with experimental data concerning melt pool size. Subsequently, by combining the experimental observations with high-fidelity simulations, we characterize the evolution of melt pools in situations with varying laser power, laser speed and laser spot size, while explaining the formation of either deep or shallow melt pools. The initial development of the melt pool under the influence of a laser heat source is further studied, with a close analysis of the factors affecting the formation of the melt pool. Finally, several keyhole modes in ceramics LPBF are identified, a discovery that proves valuable for enhancing the quality of manufactured structures.

Keywords: Laser powder bed fusion, Synchrotron X-ray, melt pool dynamics, Smoothed particle hydrodynamics

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Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PREDICTION OF DEPOSITION EFFICIENCY IN COLD SPRAY ADDITIVE MANUFACTURING USING MULTIPHYSICS AND MULTISCALE COMPUTATIONAL MODELLING, DATA-DRIVEN MODEL AND EXPERIMENTAL VALIDATIONS

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ABSTRACT

In the realm of Cold Spray Additive Manufacturing (CSAM), metal powder particles are propelled by pre-heated, high-pressure gas through a converging-diverging nozzle, reaching velocities beyond the critical range of 500m/s to 1000m/s, depending on the material type. This acceleration results in the particles impacting the substrate, allowing for material deposition and the construction of parts at a high volume rate. A key metric in CSAM, Deposition Efficiency (DE), plays a pivotal role in determining the quality and production costs of the process. DE can be influenced by various process parameters including gas pressure, pre-heating temperature, nozzle design, nozzle impingement angle, powder size distribution and more. Experimental data has shown that DE significantly affects the properties of the deposited materials, such as microstructures (including grain size and dislocation densities), hardness, porosity, and adhesive and cohesive bonding strength. To gain a comprehensive understanding of the factors influencing DE and to enhance the predictability and control of DE in CSAM processes, we have developed a multiphysics and multiscale computational modeling and simulation platform. This includes the utilization of Molecular Dynamics and Finite Element Method (FEM) modeling for single particle impact simulations to fundamentally understanding bonding mechanism and establish bonding criteria in CSAM. Furthermore, a data-driven model has been constructed based on the bonding criteria, enabling the identification of bonding and rebounding scenarios for individual particles varying in size, temperature, and velocity. The dynamics of gas flow, as well as the velocity and temperature of tens of thousands of in-flight particles, are studied using a multiphase Computational Fluid Dynamics (CFD) model, further enhanced by a serial CFD-FEM coupling model for more accurate particle temperature analysis. This integration of the data-driven model with CFD simulation results allows for the prediction of DE under various CSAM process conditions. To validate the model's accuracy, experiments were conducted, focusing on in-flight particle velocities and the DE of Ti-64 CSAM processes. The impact of DE on deposit properties such as surface morphology, porosity, and residual stresses has been illustrated through both computational modeling and experimental studies, highlighting its crucial role in CSAM.

Machine learning and multiscale modeling for complex materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MACHINE LEARNING MODEL FOR CORRELATING MICROSTRUCTURAL FEATURES AND MACROSCOPIC PROPERTIES OF HETEROGENEOUS COMPOSITES

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ABSTRACT

In the traditional micromechanics context, the size and volume fraction of inclusions in heterogeneous composites are considered the primary microstructural parameters for controlling macroscopic properties, rather than other factors. Challenges persist in accurately predicting effective properties due to a limited understanding of extensive multi-scale microstructural data using micromechanics-based methods such as homogenization and finite element analysis.
In this research, both supervised and unsupervised learning approaches are employed to explore the limits of artificial intelligence comprehension. In the case of supervised learning, analysis of scanning electron microscope (SEM) images of nickel-based superalloys from a high-throughput experiment involves defining 23 microstructural descriptors to correlate with the hardness. Subsequently, 10 descriptors are selected to reduce the computational cost of the deep neural network (DNN) with the support of the shallow neural network (SNN). Additionally, in order to enhance DNN accuracy, new training sets are proposed by incorporating these 10 descriptors along with two additional ones: area distribution and one heat treatment parameter - cooling rate. In conclusion, it is demonstrated that the supervised learning approach surpasses the predictive capabilities of existing physics-based constitutive models.

In the case of unsupervised learning, the prediction of the effective thermal conductivity of thermal insulation composite materials is achieved through the utilization of a convolutional neural network (CNN). The CNN model is trained and validated using fibrous and particulate composites images generated from numerical approaches as input data and the conductivities predicted by the Lattice Boltzmann Method (LBM) as output data. Subsequently, the CNN predictions are compared to experimental results as well as those obtained from analytical and computational micromechanics methods. It is worth noting that the proposed CNN model demonstrates accurate prediction of the thermal conductivity for materials featuring novel microstructures that were not part of the training set.

In summary, harnessing artificial intelligence to capture the scattering characteristics of heterogeneous materials enables both DNN and CNN models to achieve more efficient predictions compared to traditional methods. This highlights the potential of machine learning in advancing materials science and expediting the development of materials with desired properties.

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hardness properties of nickel-based superalloys, Journal of Materials Research and Technology, 9(6), 14467-14477, 2020.

Recent advances on interfaces dynamics modeling and simulation
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GENERAL NUMERICAL FRAMEWORK TO DERIVE STRUCTURE PRESERVING REDUCED ORDER MODELS FOR THERMODYNAMICALLY CONSISTENT REVERSIBLE-IRREVERSIBLE PDES

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ABSTRACT

In this presentation, we propose a general numerical framework to derive structure-preserving reduced-order models for thermodynamically consistent PDEs. Our numerical framework has two primary features: (a) a systematic way to extract reduced order models for thermodynamically consistent PDE systems while maintaining their inherent thermodynamic principles and (b) a strategic process to devise accurate, efficient, and structure-preserving numerical algorithms to solve the forehead reduced-order models. The platform's generality extends to various PDE systems governed by embedded thermodynamic laws. The proposed numerical platform is unique from several perspectives. First, it utilizes the generalized Onsager principle to transform the thermodynamically consistent PDE system into an equivalent one, where the transformed system's free energy adopts a quadratic form of the state variables. This transformation is named energy quadratization (EQ). Through EQ, we gain a novel perspective on deriving reduced-order models. The reduced order models derived through our method continue to uphold the energy dissipation law. Secondly, our proposed numerical approach automatically provides numerical algorithms to discretize the reduced-order models. The proposed algorithms are always linear, easy to implement and solve, and uniquely solvable. Furthermore, these algorithms inherently ensure the thermodynamic laws. Our platform offers a distinctive approach to derive structure-preserving reduced-order models for a wide range of PDE systems abiding by thermodynamic principles.

ELECTROHYDRODYNAMIC EFFECTS ON VISCOELASTIC DROPLET DEFORMATION IN SHEAR FLOWS

Jiachen Zhao[1], Vedad Dzanic[1], Zhongzheng Wang[1] and Emilie Sauret[1]*

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ABSTRACT

Abstract

The droplet-based microfluidic technologies in a confined shear flow configuration have evolved rapidly in the past decade and have shown tremendous potential in many industrial and commercial applications, such as food processing, pharmacy, and materials synthesis [1]. For many of these applications, the droplet exhibits non-Newtonian viscoelasticity, whose dynamical behaviour differs significantly from the Newtonian counterpart. The size and morphology of droplets play a crucial role in determining the mechanical properties and rheology of the resulting system. Therefore, an efficient and effective manipulation of the droplet size and morphology is of paramount importance to ensure accurate control over the dynamics of the process. It has been shown that additional stresses can be generated at the fluid interface in the presence of an electric field (electrohydrodynamics) [2], thereby significantly altering the flow behaviours. In this study, the dynamics of viscoelastic droplets under the combined action of electric field and shear flow are investigated by using a hybrid lattice Boltzmann model (LBM) and finite difference method (FDM), where the hydrodynamic field is simulated by LBM and the electric and polymer field (viscoelasticity) are solved by FDM. Both the droplet and the surrounding medium are considered to be leaky dielectric fluids. The effects of the conductivity and permittivity contrast between the fluids and the electric field strength on the viscoelastic droplet deformation and morphology are studied. The results show that in the presence of an external electric field, the deformation of the droplet can be suppressed or promoted, and the droplet inclination angle can be aligned or opposite to the shear flow direction depending on the electrical properties of the two fluids.

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Microstructures of chemically complex materials and their impacts on material properties from multiscale simulations
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DYNAMICS AND HETEROGENEITY OF PARTICLE NETWORK IN COMPOSITE ELECTRODES OF LI-ION BATTERIES

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ABSTRACT

We use a data-driven approach to assess the heterogeneous electrochemistry and mechanics in composite cathodes. We visualize the morphological defects at multi-scales ranging from the macroscopic composite, particle ensembles, to individual single particles. Particle fracture and interfacial debonding are identified in a large set of tomographic data. The mechanical damage of active particles is highly heterogeneous. The difference originates from the polarization of the electrolyte potential, various local conducting environments, and thus the non-uniform distribution of the activation energy for the charge transfer reaction. We model the kinetics of intergranular fracture and interfacial degradation to assess the heterogeneous mechanical damage in composite electrodes using microstructure-informed mechanics modeling. We quantify the influence of the mechanical damage on the metrics of battery performance. More interestingly, the interfacial failure reconstructs the conductive network and redistribute the electrochemical activities that render a dynamic nature of electrochemistry and mechanics evolving over time in the composite electrodes.

Next-generation numerical methods for coupled multiphysics problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A UNIFIED MIXED METHOD FOR THE FLUID-STRUCTURE INTERACTION

Lina Zhao[*1]*

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ABSTRACT

In this talk we propose and analyze a staggered DG method free of stabilization in stress-velocity formulation for fluid-structure interaction. A unified formulation is employed for the Stokes equations and the elastodynamic equations. The symmetry of stress is strongly imposed and equal order polynomials are employed for all the variables. The proposed scheme yields divergence-free fluid velocity. In particular, the transmission conditions can be incorporated naturally without resorting to additional variables or Nitsche-type stabilization owing to the bespoke construction of the discrete formulation. Moreover, the dynamic coupling interface condition is satisfied strongly in the definition of the approximation space. Optimal convergence for all the variables can be obtained. Furthermore, the pressure-independence, and the robustness with respect to fluid viscosity and the Lam\'{e} constants are investigated. The proposed scheme is hybridizable and the globally coupled unknowns only involve the normal trace of stress. Importantly, the resulting matrix is shown to be symmetric positive definite, rendering the scheme computationally attractive. Several numerical experiments are presented to verify the proposed theories.

Fluid-structure interaction in interface and moving boundary problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

THREE-LAYER HELE-SHAW PROBLEM DRIVEN BY A SINK

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ABSTRACT

We investigate a sink-driven three-layer flow in a radial Hele-Shaw cell performing numerical simulations. The three fluids are of different viscosities with one fluid occupying an annulus-like domain, forming two interfaces with the other two fluids. Using a boundary integral method and a semi-implicit time stepping scheme, we alleviate the numerical stiffness in updating the interfaces and achieve spectral accuracy in space. The interaction between the two interfaces introduces novel dynamics leading to rich pattern formation phenomena, manifested by two typical events: either one of the two interfaces reaches the sink faster than the other (cusp-like morphology) or they touch each other (interface merging). In particular, the inner interface can be wrapped by the other to have both scenarios. We find that multiple parameters contribute to the dynamics including the width of annular region, the location of the sink, and the mobilities of the fluids.

Computational geomechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

HIERARCHICAL MULTISCALE MODELING OF FLUID-SOIL INTERACTIONS FOR LARGE-DEFORMATION PROBLEMS

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ABSTRACT

Large deformation problems in fluid-saturated granular media are of significant concern in areas such as natural geohazards and engineering applications. The multiscale nature of granular media has gained increasing recognition with advancements in experimental and numerical tools. In this study, we propose a novel multiscale hydro-mechanical approach that couples the double-point Material Point Method (MPM) with the Discrete Element Method (DEM). To capture the complexities of the system, we employ an explicit double-point MPM with two-phase media. This approach enables the description of soil-water interactions, the transition from free water to groundwater, as well as the fluidization and sedimentation behavior of soil. Additionally, DEM is utilized to simulate the response of a representative volume element (RVE), which acts as a surrogate for the conventional constitutive model at a material point. This allows for adaptability to complex loading conditions. To validate the accuracy of our method, we compare the results to analytical solutions of consolidation theory. Subsequently, the method is employed to simulate various dynamic experiments, including the collapse of submerged granular-liquid mixtures and the generation of water waves caused by the collapse of dry granular materials into water. Furthermore, we enhance the computational efficiency of the numerical simulations by employing hybrid OpenMP and GPU-based parallelization. This approach offers an efficient and effective pathway for addressing large-deformation problems involving complex hydro-mechanical coupling in granular media. Overall, our proposed multiscale, hydro-mechanical approach, combining the double-point MPM with DEM, demonstrates promising capabilities in accurately capturing and simulating large-deformation phenomena in fluid-saturated granular media.

Fracture, damage and failure mechanics of cementitious materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPERIMENTAL AND NUMERICAL STUDY ON CRACK PROPAGATION OF CONCRETE AFTER LOW-CYCLE RECIPROCATING LOADING

Wenhu Zhao[*1] and Yi Li*[1]

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ABSTRACT

Concrete structures usually contain cracks or micocracks that directly weaken concrete strength and structure's stability. To fully understand the fracture behaviour of concrete with initial micocracks or damage, a series of concrete specimens are split using an improved wedge splitting device after low-cycle reciprocating loading. Due to the additional springs on the device, the complete stress-strain curves representing concrete fracture are measured and recorded, including the evolution of micro-cracks, damage accumulation, and ultimate fracture stages. Compare to the results of normal tests, the differences on the fracture toughness and fracture energy are analyzed and calculated with the double-K fracture model. The measured values of the initiation force, the initiation toughness and the unstable toughness increase slightly because the weaker bond zones have accomplished fracture, and the rest performance of concrete specimen is mainly determined by the properties of coarse aggregates. The results show that the reciprocating loading changes the failure pattern and that more failures occur around the coarse aggregates, causing the relative ratio up to over 160%. Meanwhile, a numerical simulation of crack propagation is carried out based on the scaled boundary finite element method (SBFEM). An equivalent stress intensity factor (eSIF) is proposed to determine the crack propagation for concrete with damage. Finally, the performance of the proposed method is verified by several numerical examples. The numerical results agree well the experimental ones and the proposed critical eSIF has high accuracy in solving the mode I and II stress intensity factors as well as simulating the internal crack growth path of materials.

Catastrophic failure mechanics and numerical modelling
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STUDY ON THE INFLUENCE OF VALLEY WIDTH DEFORMATION ON THE SAFETY OF HIGH ARCH DAM CONSIDERING UNSATURATED SEEPAGE

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ABSTRACT

Abstract: The effect of valley width deformation during the initial impoundment stage on the subsequent working behavior and the long-term safety of an arch dam has become an increasingly important challenge faced by dam engineering and academia. This study aims to analyze the sensitivity of valley width deformation to the absorption curve of fractured rock mass to address the challenge of valley width reduction during impoundment of the Jinping Ⅰ arch dam in China. The methods of unsaturated seepage analysis theory and nonlinear finite element numerical analysis were applied to study the law of valley width deformation during unsaturated seepage process. The influence of valley width deformation on the displacement and stress of the dam was analyzed. The results showed that the slope on both sides of the valley deformed towards the center under the action of the unsaturated seepage field. The deformation of valley width upstream exceeded that downstream. The valley width deformation increased with an increasing elevation
of the water level, and maximum valley width reduction occurred in the saturated seepage field. The distribution of displacement and stress of the dam changed little during the unsaturated seepage process. However, the maximum longitudinal displacement and the minor principal stress of the dam decreased gradually with increasing elevation of the water level. There was a gradual increase in the major principal stress. However, the valley width deformation resulting from the seepage field had a limited effect on the displacement and stress of the dam, which would not affect the overall stability of the dam.

Key words: unsaturated seepage; absorption curve; valley width deformation; high arch dam

Battery modeling and computation: From material to device
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHASE-FIELD FORMULATION FOR PREDICTING VOID EVOLUTION AT THE LI-ELECTROLYTE INTERFACE IN ALL-SOLID-STATE BATTERIES

Ying Zhao[1], Emilio Martinez-Paneda[2] and Runzi Wang[2]*

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ABSTRACT

All-solid-state batteries are among the most promising energy storages, because they use unflammable solid electrolyte in substitution of organic liquid electrolytes, thus reducing safety hazards. Moreover, they can potentially allow for the employment of Li metal electrode that can significantly enhance the energy densit. However, void and dendrite formation at the interface between the Li-metal anode and the solid electrolyte are hindering the viability of all-solid-state Li-metal batteries.

In this presentation, we develop a phase-field formulation for predicting void evolution in the Li metal electrode during the charge and discharge of all-solid-state battery cells [1]. This formulation can predict vacancy annihilation and nucleation, and track of the void-Li metal interface. This is coupled with a viscoplastic description of Li deformation, to capture creep effects, and a mass transfer formulation accounting for substitutional (bulk and surface) Li diffusion and current-driven flux. Moreover, we incorporate the interaction between the electrode and the solid electrolyte, resolving the coupled electro-chemical-mechanical problem in both domains. This enables predicting the electrolyte current distribution and thus the emergence of local current ‘hot spots’, which act as precursors for dendrite formation and cell death. The theoretical framework is numerically implemented, and single and multiple void case studies are carried out to predict the evolution of voids and current hot spots as a function of the applied pressure, material properties and charge (magnitude and cycle history). For both plating and stripping, insight is gained into the interplay between bulk diffusion, Li dissolution and deposition, creep, and the nucleation and annihilation of vacancies. The model is shown to capture the main experimental observations, including not only key features of electrolyte current and void morphology but also the sensitivity to the applied current, the role of pressure in increasing the electrode–electrolyte contact area, and the dominance of creep over vacancy diffusion.

Reference

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Machine learning and multiscale modeling for complex materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN EFFICIENT MULTISCALE SIMULATION FRAMEWORK OF ADS COMPOSITE FUEL BY INCORPORATING AN INTERPRETABLE DEEP-LEARNING-BASED SWELLING MODEL

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ABSTRACT

Numerical analysis of nuclear fuel composites is a classic engineering problem with multiphysics and multiscale nature. Owing to the complicated mechanical, thermal effects, and multiscale irradiation damage effects, the modeling framework usually suffers from limited applicability in engineering practice. In this study, a novel framework for the multiscale analysis of the ADS (Accelerated driven system) fuel composite is proposed, in which a deep learning surrogate is employed to describe the hydrostatic-pressure-dependent swelling behavior, circumventing the difficulties associated with conventional approaches. The surrogate model was trained by a Long Short-Term Memory (LSTM) deep learning model that excels at processing the sequential nature of the swelling evaluation with irradiation burnups. The model was further incorporated within the stress update algorithm in UMAT/ABAQUS. During the FE solution, the surrogate receives the key history features of temperature, hydrostatic pressure, and swelling deformation at the Gauss integration points and returns the predicted swelling strain to advance the computation. The applicability and capacity of the machine-learning-assisted framework were demonstrated by analyzing three simulation cases, in which different loading conditions and irradiation effects were considered. It was shown that the framework can reproduce satisfactory solutions without resorting to any constitutive theory. Furthermore, the use of the DL model not only avoids the stress integration of the conventional FE analysis but also leads to better computational efficiency.

Uncertainty quantification and reliability analysis in engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ROBUST TOPOLOGY OPTIMIZATION FOR STRUCTURES WITH SPATIALLY BOUNDED GEOMETRIC UNCERTAINTY

Jing Zheng[*1] and Chao Jiang[1]*

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ABSTRACT

In structural topology optimization design, a series of robust topology optimization methods have been developed considering the uncertainties related to material properties and applied loadings. In addition, manufacturing errors or measurement errors often lead to the uncertainty of structure boundaries. The structural design may be very sensitive to the small fluctuation of the boundary. On the one hand, it is difficult to obtain the probability distribution of the boundary uncertainty due to the high-cost experiment or limited data. On the other hand, structural boundary uncertainty is generally uncertain but spatially bounded. In this work, the interval field is used to measure the geometric uncertainty, and an efficient robust topology optimization method based on Chebyshev polynomial expansion is developed. Firstly, the boundary disturbance of the structure is described by modelling the projection threshold variable in the Heaviside filter as an interval field, and a robust topology optimization model under the worst case is then constructed. Secondly, based on the interval KL (Karhunen-Loève) expansion, the interval field is approximately discretized into finite interval variables, and the robust objective function and constraint are evaluated using the Chebyshev polynomial expansion method. Thirdly, the sensitivities of the robust objective function and constraint with respect to the design variables are derived, and the gradient-based optimization algorithm is used to update the topology design variables. The analysis results of numerical examples show that the geometric uncertainty fluctuation of the structural boundary has an important impact on the structural performance. Compared with the topology optimization design under the deterministic boundary, the robust topology optimization design considering uncertainty has better robustness when considering the fluctuation of the structural boundary.

Topology optimization for additively manufactured metamaterials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOPOLOGY OPTIMIZATION-BASED DESIGN METHOD FOR LOW-PROFILE HIGH-GAIN ENDFIRE CIRCULARLY POLARIZED ANTENNAS

Junfeng Zheng[*1], Qi Wang[1], Renjing Gao[1] and Shutian Liu[1]*

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ABSTRACT

Metallic antennas with excellent properties (single feed, broadband, endfire radiation, high gain, and circularly polarized) are attractive for modern wireless communication systems. However, the complex radiation is extremely challenging for conventional parameter optimization-based design methods. In particular, when the profile of the antenna is lowered, it is difficult to achieve circularly polarized waves because of the mismatch between the profile and cross-sectional dimensions, which imposes stringent requirements on the design of the antenna configuration. To overcome this difficulty, a topology optimization approach is introduced for the design of a low-profile, high-gain end-fire circularly polarized antenna. The objective of the design problem is to maximize the gain of the metallic antenna while maintaining a circularly polarized wave around the direction of the endfire radiation. The material distribution approach is adopted to search for the optimal distribution of metal materials, and the material resistance is chosen to be interpolated with the design variables to differentiate between metallic conductors and nonconductors. Since the metallic antenna radiation performance is sensitive to the gray elements, to obtain a discrete solution, the design variable is iteratively projected using a smoothed Heaviside projection function during the optimization process. For the zig-zag boundary and the leftover gray elements, a Bessel curve-based shape optimization approach is proposed to reoptimize the topological conceptual configuration, thus antenna with smooth boundaries can be obtained.

Advances in computational biomechanics and mechanobiology
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

SPECIMEN-SPECIFIC FINITE ELEMENT MODELLING OF CARTILAGE MECHANICS: A NEW PARADIGM IN LINKING TISSUE ULTRASTRUCTURE TO ITS MICROMECHANICS

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ABSTRACT

The architecture of collagen network plays the dominant role in determining the biomechanical behaviour of articular cartilage, which exhibits strong directionality and anisotropy [1]. Several theoretical material models have been developed to study the micromechanics of cartilage [2], but few have been capable of capturing the specimens-specific heterogeneity in the organisation of the fibrous network across multiple length scales. Polarisation-resolved Second Harmonic Generation (pSHG) microscopy is an emerging technique that allows the principal orientation and the molecular order (dispersion) of collagen fibre networks to be probed below the optical diffraction limit [3]. These data await to be incorporated into image-based finite element (FE) simulations to study cartilage mechanics in a specimen-specific manner. This study aims to establish a framework for combining the collagen network architecture quantified by pSHG and FE analysis, to establish a link between the ultrastructural parameters and the micromechanics of the tissue, therefore inferring the mechanobiological environments of cells within. A multiphasic material model was developed to govern the interaction among different major constituents, including the non-fibrillar extracellular matrix (ECM), the fibrillar collagen network, the osmotic pressure, and the interstitial fluid. The pixel-based fibril orientation information from pSHG images was then assigned to the elemental material properties in the FE model. The fibrillar stress and pore pressure were quantified for the cartilage in the sagittal plane which had three zones of distinct collagen organization. Under a uniaxial compression loading, three different zones respond differently. It is not only due to the different fibrillar orientation, but also because the deformation of the chondrocyte varies across three zones. In addition, the mechanical response showed discrepancies between the territorial and inter-territorial matrix. The cartilage model presented in this study incorporated the local fibrillar orientation information to link ultrastructure to its micromechanics, and results implied that heterogeneity of fibrillar structure affects the local biomechanical behaviours of cartilage, not revealed in the theoretical models before.

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Data-driven modeling and design of materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

UNIFYING THE DESIGN SPACE AND OPTIMIZING LINEAR AND NONLINEAR TRUSS METAMATERIALS BY GENERATIVE MODELING

Li Zheng[*1], Konstantinos Karapiperis[1], Siddhant Kumar[2] and Dennis Kochmann[1]*

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ABSTRACT

The rise of machine learning has fueled the discovery of new materials and, especially, metamaterials—truss lattices being their most prominent class. While their tailorable properties have been explored extensively, the design of truss-based metamaterials has remained highly limited and often heuristic, due to the vast, discrete design space and the lack of a comprehensive parameterization. We here present a graph-based deep learning generative framework, which combines a variational autoencoder and a property predictor, to construct a reduced, continuous latent representation covering an enormous range of trusses. This unified latent space allows for the fast generation of new designs through simple operations (e.g., traversing the latent space or interpolating between structures). We further demonstrate an optimization framework for the inverse design of trusses with customized mechanical properties in both the linear and nonlinear regimes, including designs exhibiting exceptionally stiff, auxetic, pentamode-like, and tailored nonlinear behaviors. This generative model can predict manufacturable (and counter-intuitive) designs with extreme target properties beyond the training domain.

Certification of simulations and model adaptation in computational science and engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STRICT UPPER AND LOWER BOUNDS ON QUANTITIES OF INTEREST FOR TRANSIENT DYNAMICS

Qisheng Zheng[*1], *Li Wang*[1] *and Jike Liu*[1]

[1]*Sun Yat-sen University*

ABSTRACT

This work proposes a guaranteed error estimator for linear transient elastodynamics, accounting for both time- and space-discretization errors. The key lies in the definition of a novel dynamic constitutive relation error formulation, which is proven to be the strict bound of the discretization error. Moreover, based on the established dynamic constitutive relation error and the goal-oriented error estimation framework, strict upper and lower bounds on quantities of interest are also obtained. Numerical examples are conducted to verify the proposed strict bounds and to explore the potential application of these bounds to adaptive time-stepping and mesh-refinement.

FRACTURE PREDICTION OF HYDROGEL USING MACHINE LEARNING AND INHOMOGENEOUS MULTISCALE NETWORK

Shoujing Zheng[1], Hao You[1], K.Y. Lam[1] and Hua Li[1]*

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ABSTRACT

Hydrogels are soft polymeric materials with promising applications in biomedical fields. Understanding their fracture behavior is crucial for optimizing device design and performance. However, predicting hydrogel fracture is challenging due to the complex interplay between material properties and environmental factors. In this study, we present a machine learning (ML) approach to predict hydrogel fracture behavior. A multiscale hydrogel fracture model is developed to generate simulation data, which is used to train a predictive neural network model. The ML model utilizes a hierarchical architecture of convolution long short-term memory units to capture spatial and temporal dependencies in the data. Model predictions are found to closely match simulation results with high accuracy, demonstrating the ability to learn complex fracture processes. Comparison of crack lengths shows the model can generalize across different material parameters. This work highlights the potential of ML for advancing the understanding of hydrogel fracture and soft matter failure. The presented approach provides an efficient framework for predicting fracture in complex materials and systems.

Advances and applications in meshfree, particle, and peridynamic methods
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

PHASE-FIELD TOTAL LAGRANGIAN MATERIAL POINT METHOD FOR FRACTURE IN SOFT MATERIALS

Yonggang Zheng[1], Zijian Zhang[1], Hongfei Ye[1] and Hongwu Zhang[1]*

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ABSTRACT

Fracture problems of soft materials under large deformation exist widely in nature and engineering areas. Predicting the facture behaviors is of great importance for the structural design and safety assessment of many soft materials based devices. However, effective and accurate prediction of these behaviors remain challenging due to the coupled nonlinear mechanical responses of large deformation, contact and fracture. To address these problems, we have recently developed an explicit phase-field total Lagrangian material point method. In this method, the phase-field model was introduced to describe the cracks and the governing equations of the dynamic system were derived via the Lagrangian equation. Considering the massive deformation of soft materials, the TLMPM discretization was then developed for the displacement and phase field governing equations. To deal with the contact during the dynamic process, a particle-based contact algorithm was also proposed for both contact and self-contact problems within the total Lagrangian framework. Furthermore, with the consideration of the weak compressibility of series soft materials, the proposed method was developed to avoid the volumetric locking for near-incompressible materials by introducing a pressure field. Several complicated problems, including the impact of a metal ball on a soft membrane, the compression of soft blocks and the out-of-plane tearing of gels were presented to illustrate the performance of the proposed method for the dynamic fracture of soft materials in practical applications. These works were supported by the National Natural Science Foundation of China (Nos. 12072062, 12072061 and 11972108).

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Computational mechanics of soft matter and machines
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GLASS COMPRESSION CREEP TEST MODELLING

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ABSTRACT

Three modelling/analysis approaches are developed to study the glass compression creep test process, including analytical analysis based on Navier-Stokes equations, viscous fluid finite element analysis (FEA) modelling and viscoelastic solid finite element analysis (FEA) modelling. It is confirmed that the three methods generate the same result under the ideal condition. Impact of process parameters, like temperature, slip condition, is studied. Viscoelastic model study shows that the viscoelasticity impacts the result only to a small scale, and only at around or sub glass transition temperature Tg.

Nanomechanics and nanoscale thermal transport for new materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VIBRATIONAL CHARACTERISTICS OF SP3 CARBON NANOSTRUCTURES

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ABSTRACT

In past years, nanoelectromechanical systems (NEMS) attract interest from broad fields. The excellent vibrational properties of low-dimensional nanomaterials are crucial, which allows the detection of minute frequency shift under external perturbations. Recently, low dimensional sp3 carbon nanostructures have attracted increasing attention, due to their unique properties.
Targeting the ultra-sensitive sensing applications, this presentation contains a comprehensive study on the vibration properties of several novel low dimensional sp3 carbon nanomaterials, such as carbon nanothreads (NTH), diamane and its analogues [1-3]. Size effect is observed in transverse free vibrations of NTHs. The modified couple stress theory (MCST) based Timoshenko beam model is utilized to quantify such effects. Based on molecular dynamics simulations and continuum mechanics model, the natural frequencies and corresponding modal shapes of diamane are investigated. The results show that the Kirchhoff plate model can reasonably predict the vibration properties of diamane. Furthermore, the vibrational characteristics of the diamane's analogue - twisted bilayer graphene with interlayer-bonding (TBGIB) are studied. It is found that the interlayer shear modulus plays an important role in the natural frequencies of TBGIBs.
This work provides a comprehensive understanding of the vibration properties of carbon nanaothreads, diamane and its analogues, which should be beneficial to the tuning of ultrasensitive nano resonators.

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Deep and machine learning methodology in the context of application to computational mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

GRAPH NEURAL NETWORKS FOR ACCELERATING THE DISCRETE ELEMENT SIMULATION OF GRANULAR FLOW

Peng Zhi[*1] and YuChing Wu*[1]

[1]*Tongji University*

ABSTRACT

Granular flow is a phenomenon widely presented in both the natural and engineering fields. Here granular materials could be either solid particles, e.g. rocks, soil, and grains, or liquid particles, e.g. mud and fresh concrete mortar. Soil landslides, particle transport, and grain accumulation have been edge-cutting hot research topics. Discrete Element Method (DEM) has been regarded as one of the most important methods to simulate granular flows and to investigate discontinuous and large deformation problems. The basic principle of DEM was to view the simulated object as consisting of discrete particles, to define specific constitutive relationships for the particles, and to study the macroscopic properties of the simulated object from a microscopic perspective based on the interactions between particles. However, DEM simulations usually consume very high computational cost for particle contact searching and detection. To accelerate the computational process of discrete element simulation, the Graph Neural Network (GNN) based deep learning model was proposed in this paper. In GNNs, graph nodes and graph edges represent the particles and their interactions. The training and testing datasets were generated using an open-source software named YADE, while the neural network model was constructed using PyTorch and Deep Graph Library (DGL). Replacing the direct calculation of particle collisions in DEM with the trained neural network model, the state of the particles at the next moment could be predicted based on the current state of the particles. It significantly increased computational speed. The proposed technique was applied in various examples, such as particle stacking and drum rotation. Its accuracy and efficiency were demonstrated to be superior to other deep learning methods. This study established a solid foundation and provided robust support for further research and applications of granular flow simulation.

Professor JN Reddy's contributions to computational mechanics - A minisymposium on the occasion of Prof. Reddy's 80th birthday
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A THERMO-CHEMO-MECHANICALLY COUPLED PERIDYNAMICS FOR INVESTIGATING CRACK BEHAVIOR IN SOLIDS

Zheng Zhong[*1]*

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ABSTRACT

In engineering applications, the phenomenon of cracking is often accompanied by a coupled multiphysics effect. Peridynamics (PD) is an effective approach for solving cracking problems, but currently, no general PD model accounts for the coupling of multiple physical fields. In this work, we develop a PD model of coupled deformation, heat conduction, species diffusion, and chemical reactions. First, we establish the equations for mass, linear momentum, and energy. Then we establish fully coupled constitutive laws that interpret the interactions between the various fields and formulate evolution equations that govern the flux of species and heat. These laws and equations are developed based on the inequality of energy dissipation and the principles of chemical kinetics. Species diffusion and chemical reactions are treated as separate processes to study their effects on the Helmholtz free energy density of solids and the subsequent formation and propagation of cracks. In addition, certain coupling coefficients are calibrated by equating the corresponding physical quantities in the PD model with those in continuum mechanics. Four specific cases are simulated to validate the model, including redistribution of vacancies in ceramics, hydrogen traps,and embrittlement in metals.

Numerical modeling of granular and multiphase flows
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

AN EFFECTIVE ALGORITHM BASED ON SIX-EQUATION DIFFUSION INTERFACE MODEL FOR SIMULATING CONDENSED PHASE DETONATION

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[2]*Institute of Applied Physics and Computational Mathematics*

ABSTRACT

We propose an effective algorithm for simulating the interaction between condensed-phase explosives and inert materials. The augmented Euler system (with an equation evolving the mass fraction), which can preserve the conservation property, is applied to model the mixture of explosive and its products, and a six-equation multi-phase diffusion interface approach is adopted to resolve the interaction between explosive mixtures and immiscible inert materials. Similar to the work of Saurel et al.[1], the Newton iteration nonlinear equation system of pressure relaxation terms is derived by combining the energy balance equation and the thermal equilibrium between explosive mixtures. And an effective root-finding process is developed by the initialization with the preliminary equation solutions. Several detonation examples are simulated to validate the robustness and efficiency of the new algorithm, and the comparisons to the algorithm based on the five-equation model[2] are also presented.

Key words: Condensed Phase Detonation, Six-Equation Model, Multiphase, Robustness, Relaxation.

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MULTISCALE MIXED METHODS WITH IMPROVED ACCURACY: THE ROLE OF OVERLAPPING AND SMOOTHING

Dilong Zhou[*1] and Luis Felipe Feres Pereira*[1]

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ABSTRACT

Multiscale mixed methods based on non-overlapping domain decompositions have been carefully studied in recent years. Linear solvers for porous media flow problems based on these methods are naturally parallelizable in multi-core computers and can handle efficiently the solution of large problems in very heterogeneous formations of interest to the industry.
Efficiency in the numerical solutions is dictated by the choice of interface spaces that are selected: the smaller the dimension of these spaces, the better, in the sense that fewer multiscale basis functions need to be computed and smaller interface linear systems need to be solved. Thus, in the solution of large computational problems, it is desirable to work with piecewise constant or linear polynomials. In these cases, it is well known that the flux accuracy, when computed in terms of fine grid solutions, is of the order of 10^-1.
In this work, we focus on the development of a practical, efficient, and accurate solver for large problems. We consider subdomains with small overlapping regions, and we introduce the concept of a smoothing step, to handle small-scale errors in the multiscale solution. Moreover, we introduce novel informed spaces for the calculation of multiscale basis functions.
Several numerical studies are presented to illustrate the good properties of the new solver. We consider initially a problem with an analytical solution followed by a careful study of two-dimensional solutions of several layers of the permeability field of the SPE 10 project.

Uncertainty quantification and reliability analysis in engineering
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A MODEL ON STRESS ANALYSIS OF ADHESIVE LAYER IN PLATED BEAM

Fen Zhou[*1]*

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ABSTRACT

The prediction of stresses in an adhesive layer is helpful in revealing the mechanism of debonding failure in plated beams. This study proposes an improved analytical model for the stress analysis of an adhesive layer in a plated beam. The beam and the soffit plate are individually modelled as a single Timoshenko sub-beam with separate rotations, while the adhesive layer is modelled as a two-dimensional elastic continuum in plane stress, which considers different adherend-adhesive interface stresses. The internal forces of the adhesive layer are assumed to satisfy the Timoshenko beam theory, and the shear deformation and bending moment of the adhesive layer can be considered. The internal forces and displacements of the adhesive layer are fully considered in the displacement compatibility equations, and deformable interfaces are assembled so that the effect of interface stresses on local deformation is captured. Based on equilibrium equations and displacement continuity, the governing differential equations of beam forces are derived, and then the analytical solutions of interface stresses and stresses along the thickness of the adhesive layer are obtained. Comparisons of the results of the finite□element analysis and the existing four-parameter model solutions show that the present model is reasonable. The influence of adhesive thickness on stress distributions in adhesive layers is also investigated.

Computational methods in environmental fluid mechanics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EXPLORING COMPLEX ENVIRONMENTAL FLOW PHENOMENA WITH THE LATTICE BOLTZMANN METHOD

Qi Zhou[*1]

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ABSTRACT

This presentation combines findings from three distinct studies, each leveraging the lattice Boltzmann method (LBM) to investigate various aspects of environmental fluid dynamics:

1. Rayleigh–Taylor instabilities under granular suspensions: The first study delves into Rayleigh–Taylor instabilities at the interface between a granular particle suspension and a clear fluid [1]. Employing a combination of lattice Boltzmann and discrete element methods, this research focuses on the instabilities' growth rate and average wave number. It examines the impact of the solid fraction of the suspension and the solid-to-fluid density ratio, shedding light on the dynamics of interfacial granular RTI and the potential of continuum-based linear stability analysis in such contexts.

2. Simulation of stratified plane Couette flows: The second study uses LBM to model stratified plane Couette flows, evaluating LBM's capacity for directly simulating wall-bounded, sheared turbulence under stable stratification [2]. The study presents a complete analysis of turbulence statistics by drawing comparisons between LBM outcomes and direct numerical simulations executed via the conventional pseudo-spectral method. It highlights the importance of selecting appropriate grid spacing in LBM to achieve accurate resolution in stratified wall-bounded turbulence scenarios.

3. Self-organization in stratified turbulence: The third study probes into the self-organization of strongly stratified turbulence, focusing on a local critical state within numerically simulated stratified turbulent flows. The approach [3] involves separating the turbulent flow field into large and small scales for an examination of energy transfer dynamics. The study delves into the possibility of flow self-organization under the influence of intense stratification, offering new perspectives on the behaviour of stratified turbulence.

The presentation aims to underscore the innovative use of LBM in environmental fluid mechanics, showcasing its versatility and effectiveness in unravelling the dynamics of fluid flows in natural and engineered systems.

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Numerical modelling of composite materials and structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

FIBER HYBRIDIZATION EFFECTS ON RESISTANCE TO REPEATED LOW-VELOCITY IMPACT OF MG-BASED FIBER METAL LAMINATES

Xia Zhou[*1], Wogayehu Worku Tegegne[1] and Guohui Qu[2]*

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ABSTRACT

In order to investigate fiber hybridization effects on repeated low-velocity impact response of novel fiber reinforced AZ31B magnesium alloy laminates (Mg-FMLs)，the theoretical and numerical analyses of single and repeated low velocity drop weight impact tests on Mg-FMLs reinforced with pure glass fiber (GF) and carbon fiber (CF) and their hybrids were conducted. The simulation predictions are also compared with the existing experimental results [1]. On the basis of the verification of the simulation model, the impact resistance of hybrid CF and GF reinforced Mg-FMLs with different layups was also simulated. This study provides a reasonable basis for the accurate evaluation of the impact behavior and performance optimization of lightweight Mg-FMLs [2].
The Mg alloy, the interfacial delamination between two neighboring layers and the fiber/epoxy composites in the fiber/AZ31B Mg laminates were modeled by using an anisotropic plastic constitutive model, an exponential cohesive zone model, and 3D Hashin failure criteria incorporated with the stiffness reduction of failed elements, respectively. In addition，the numerical analyses of low-velocity impact for different fiber/Mg laminates were carried out by using ABAQUS /Explicit with a user-defined subroutine VUMAT to predict the dynamic impact response and delamination as well as damage evolution rules under conditions of different low-velocity impact loadings. Meantime, the variations of impact force, deformation and energy absorption with impact number for various Mg-based FMLs were also analyzed.

The results show that impact response predictions of GF/Mg alloy laminates are in agreement with the existed experimental data under different impact energies. The repeated low-velocity impact resistance of CF reinforced Mg-FMLs can be improved by the incorporation of GF at suitable lay-up locations. For the hybrid fiber reinforced Mg-FMLs with 3/2 lay-up configuration, the hybrid laminates have the strongest resistance to repeated impact when the glass fibers are laid at the second layer of the hybrid fiber composite layers due to the larger impact contact force, smaller deformation deflection and proper energy absorption as well as higher delamination resistance.

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Modeling mechanics of materials with voids
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VOID AND HELIUM BUBBLE INTERACTIONS WITH DISLOCATIONS IN AN FCC STAINLESS STEEL ALLOY: ANOMALOUS HARDENING AND VOID CROSS-SLIP LOCKING

Ryan B. Sills[1], Xiaowang Zhou[2] and Michael E. Foster[2]*

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ABSTRACT

The critical stress for cutting of a void and He bubble by edge and screw dislocations has been determined for FCC Fe0.70Cr0.20Ni0.10—close to 300-series stainless steel—over a range of bubble spacings, diameters, pressures, and glide plane positions. The results exhibit anomalous trends with spacing, diameter, and pressure when compared with classical theories for obstacle hardening. These anomalies are attributed to elastic anisotropy and the wide extended dislocation core in low SFE metals, indicating that caution must be exercised when using perfect dislocations in isotropic solids to study void and bubble hardening. In many simulations with screw dislocations, cross-slip was observed at the void/bubble surface, leading to an additional contribution to strengthening. We refer to this phenomenon as void cross-slip locking, and argue that it may be an important contributor to void and bubble hardening.

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Applications of shape optimization in complex engineering problems
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

RESEARCH ON HEAT DISTRIBUTION DESIGN OF CARBON CERAMIC BRAKE DISCS AND SHAPE OPTIMIZATION OF RIB FOR HIGH-SPEED TRAIN

Yili Zhou[*1] and Shuguang Yao*[1]

[1]*Central South University*

ABSTRACT

High speed and lightweight are the development trends of high-speed trains in the world. Air braking technology is the last line of defense to ensure the safety and reliability of trains. The complex working environment and huge braking power put forward higher requirements for brake disc configuration and material. Carbon-ceramic composite materials have the characteristics of large specific heat capacity, thermal shock resistance, lightweight and high temperature resistance, and are considered to be high-performance friction materials. By imitating the distribution of animal and plant nutrients transportation pipelines, a carbon-ceramic composite brake disc structure with #-shaped heat dissipation ribs was designed that take into account the anisotropy of the thermal conductivity of carbon-ceramic composite materials. The branched rib structure realizes rapid heat transmission in the disc material, thereby achieving high efficiency and uniform temperature distribution, prevents the concentration of heat generated by friction, which can reduce the maximum temperature value under braking conditions. Then combined with the shape optimization and size optimization design of the local heat dissipation ribs of the brake disc, Further research on the uniform temperature performance and pump wind effect under emergency braking conditions of 400km/h was carried out. The Kriging model was used to analyze the different outlet angle, inlet angle and number of the cooling ribs in the same reference flow field. By comprehensively considering parameters such as the average maximum temperature, convection heat transfer coefficient, and pumping efficiency, an optimal design that balances cooling efficiency and aerodynamic loss is obtained.

Uncertainty quantification in structural dynamics
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

ANALYTICAL SOLUTION OF THE GENERALIZED PROBABILITY DENSITY EVOLUTION EQUATION WITH MULTIDIMENSIONAL RANDOM VARIABLES: THE CASE OF EULER-BERNOULLI BEAM

Yongfeng Zhou[*1] and Jie Li*[1]

[1]*Tongji University*

ABSTRACT

The analytical solution of the generalized probability density evolution equation not only holds significant theoretical value, but also serves the purpose of validating numerical solutions and subsequently calibrating the errors in numerical algorithms. In a general sense, the generalized probability density evolution equation has an analytical solution. However, limited by its form - multidimensional integration containing Dirac functions, the analytical solution for this equation is limited to a small number of simple systems under a single random variable. Therefore, according to the basic idea of converting multidimensional integration into one-dimensional integration, taking the Euler-Bernoulli simply supported beam as an example, the analytical solution of the generalized probability density evolution equation corresponding to the mid-span displacement response of the beam under forced vibration is derived. The solutions include those under non-stationary and non-Gaussian random excitations (involving 2-dimensional random variables) as well as those considering both the randomness of excitations and structural parameters (involving 2-dimensional, 4-dimensional and 5-dimensional random variables, respectively). The analysis results indicate that the real evolution of probability density is a highly intricate process. This advancement can provide a foundational aspect for further in-depth research into the theory of probability density evolution.

Recent advances in computational fracture mechanics and failure analysis
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

APPLICATION OF COMPUTATIONAL DAMAGE MECHANICS IN THE DEVELOPMENT OF DOWNHOLE COMPLETION TOOLS

Zhong Zhou[*1], Allan Zhong[1], Gordon McLeary[1] and Stephen Maddux[1]*

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ABSTRACT

Material modelling is crucial for predicting material behaviors and for improving the robustness of product designs. Specifically, the incorporation of damage mechanics and fracture mechanics principles through finite element analysis (FEA), has become indispensable in achieving these objectives for many applications. Accurately predicting material damage is difficult especially in the complex conditions encountered in the energy industry.

Damage mechanics provides insights into the evolution of material degradation. The widely adopted Johnson-Cook plasticity and damage model offers a sophisticated representation of material response under complex loading conditions and enables a realistic simulation of both plastic deformation and damage accumulation. On the other hand, fracture mechanics focuses on the initiation and propagation of cracks, a critical aspect in predicting failure in engineering applications.

In the context of oil and gas well completion tool design, we often deal with release mechanism where controlled failure is desirable. The traditional approach uses iterations of engineering calculations and physical tests. FEA is a powerful virtual testing ground, allowing for the numerical study of the intricate interplay between material properties, geometric complexities, and loading conditions. A Johnson-Cook damage model for ductile fracture is integrated into the nonlinear FEA, which enables the visualization of stress distribution, potential failure modes, and associated failure mechanisms. This analysis enables an improved design.

This work presents two cases studies demonstrating the effectiveness of this numerical method in tool design for the energy industry. The first study involves the design of a 6061-T6 aluminum shear pin. FEA predicted a shear value below the target load and this prediction aligned closely with test data. FEA, confirmed with test results, recommended decreasing the shear pin's inner diameter to achieve the desired load. The second study investigated the design upgrade of a retention U-Clip. The Johnson-Cook plasticity and damage model constants of 22Cr stainless steel were calibrated using material test data. FEA was validated against component test results from earlier designs, revealing the failure mechanism, and yielding identical failure load as the test. The validated FEA was used to optimize a new design for a higher failure load, meeting the upgraded operation conditions.

In summary, the synergistic application of damage mechanics, fracture mechanics, and FEA in product development provides a holistic understanding of material responses to real-world operating conditions. This approach reduces development time and costs by offering virtual insights into material behavior and failure modes, enabling more efficient and optimized product designs.

Geometric mechanics formulations and structure-preserving discretizations for continuum mechanics and kinetic models
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

VISCOUS FLOW OF EVOLVING FILM WITH ARBITRARY SHAPE AND TOPOLOGY

Cuncheng Zhu[*1], Albert Chern[1] and David Saintillan[1]*

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ABSTRACT

The dynamics of evolving fluid films in the viscous Stokes limit is relevant to various applications, such as the modeling of lipid bilayers in cells. While the governing equations were formulated by Scriven in 1960, solving for the flow of a deformable viscous surface with arbitrary shape and topology has remained a challenging task. In this study, we present a straightforward discrete model based on variational principles to address this long-standing problem. The contribution is two-fold. First, we replace the classical equations, which are expressed with tensor calculus in local coordinates, with a simple coordinate-free, differential-geometric formulation. This allows us to gain a fundamental understanding of the underlying mechanics. For a general embedded surface, the velocity field is a section of the pullback bundle from the tangent bundle of the ambient space via the embedding. Through the pullback connection, the strain rate tensor is derived from the derivative of the velocity field. This coodinate-free abstraction directly leads to a discretization for the strain rate tensor on discrete meshes. Second, we construct a discrete analogue of the system using the Onsager variational principle, which, in a smooth context, governs the flow of a viscous medium. According to this principle, the velocity of the viscous film minimizes a dissipation measure known as the Rayleighian, which is a function of the strain rate tensor. In the discrete setting, instead of term-wise discretizing the coordinate-based Stokes equations, we construct a discrete Rayleighian for the system and derive the discrete Stokes equation via the variational principle. This approach results in a standard linear saddle-point problem that can be efficiently solved using the augmented Lagrangian method.

A NEW FINITE ELEMENT METHOD FOR SIMULATING WAVE PROPAGATION ON GRAPHENE SHEETS

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[2]Portland State University
[3]The University of Texas at Austin

ABSTRACT

This presentation introduces an innovative variational approach tailored for simulating the propagation of surface plasmon polaritons on graphene surfaces. The methodology treats graphene as a current-conducting thin sheet, employing an effective conductivity model. For the first time, a novel finite element time-domain method is proposed and analyzed specifically for solving this graphene model. The presentation includes rigorous demonstrations of discrete stability and error estimations for our method. Additionally, numerical findings are showcased to highlight the efficacy of this graphene-based model in accurately simulating the propagation of surface plasmon polaritons on graphene sheets.

Advances in damage & fracture modeling of multiphysics materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A DAMAGE MODEL OF COUPLED SWELLING AND LOAD-INDUCED DEFORMATIONS IN DOUBLE-NETWORK HYDROGELS AND ITS APPLICAITON ON BUCKLING ANALYSIS

Pingping Zhu[*1] and Zheng Zhong*[1]

[1]*Harbin Institute of Technology*

ABSTRACT

Double-network (DN) hydrogels have attracted a most attention among various synthetic tough hydrogels. As high load-bearing candidates, the Mullins effect and buckling instability are two frequent phenomena that may occur simultaneously in slender DN hydrogel structures. The swelling/deswelling degree of the DN hydrogel affects the coupling phenomena. A deep understanding of the interplay between these behaviors is essential. We propose a physically based damage constitutive model for a DN polymer under water-diffusion equilibrium and cyclic loadings. By fitting the experimental data of a freely swollen DN hydrogel under cyclic compression, the model shows good capability in capturing the Mullins effect and the swelling ratio. Based on the damage constitutive model and determined parameters, we investigate the Mullin effect on the buckling instability of DN hydrogel beams. Via the analytical formula of incremental modulus, we depict the global stability diagrams of the virgin DN hydrogel beam and damaged DN hydrogel beams with five historically compressive stretches. The influences of stress softening, strain stiffening and chemical potential on buckling conditions for compressive stress and slenderness ratio are thoroughly analyzed. It is found that the stress softening is dramatically against the stability of the beam, but the strain-stiffening effect would conversely help widen the stable range. Besides, it sees that a DN gel beam immersed in a sufficient low chemical potential environment has better buckling stability. These theoretical results are valuable in the preparation and structural design of DN hydrogels for repeated use purpose.

Advanced computational modelling of wood, wood-based products, bio-composites, and timber structures
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEVELOPMENT OF HIGH-STRENGTH WOODEN PALLETS UTILIZING LOCAL TIMBER FROM EHIME PREFECTURE

Xia Zhu[1], Akira Ochi[1], Tsubasa Kaneko[1], Daiki Ito[2] and Hiromichi Toyota[1]*

[1]Ehime University
[2]Ito Wood Co., Ltd.

ABSTRACT

In this study, we focus on developing a new pallet structure utilizing Hinoki and Sugi woods from Ehime Prefecture, aiming to achieve a strength comparable to that of the foreign Bay Pine. The main goal is to design a pallet that balances high strength and rigidity with cost-effectiveness. We conducted tests on single-sided, two-way entry flat pallets, conforming to the JIS 0604-1989 standard [1], using Bay Pine for the standard pallets and the local woods for the new design. The pallets measured 1100mm by 1100mm by 144mm and had a maximum load capacity of 2 tons. Through bending and compression tests adhering to JIS Z 0602 – 1988 standards [2], we assessed the strength and rigidity of both the conventional and new pallet types. Additionally, considering the anisotropy inherent in wood's structure [3], we performed a finite element analysis, incorporating custom calculation codes for elastoplastic analysis. This led to a proposed pallet structure that improved bending strength and rigidity, as well as leg compressive strength and rigidity, validated through pallet testing. The findings indicate that the new pallet design, leveraging local timber, is effective in terms of strength and cost, contributing to the advancement of regional forestry.

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Multiscale computational homogenization for bridging scales in the mechanics and physics of complex materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MACHINE-LEARNING-BASED ASYMPTOTIC HOMOGENISATION AND LOCALISATION AND DESIGN OF SPATIALLY-VARYING LATTICE CONFIGURATION

Yichao Zhu[*1]*

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ABSTRACT

In this talk, we introduce a general framework, with the use of traditional asymptotic homogenisation approaches and the emerging machine learning tools, for the (CAD-inspired) representation, (CAE-inspired) analysis and (CAD-CAE integrated) design of smoothly-varying lattice configurations. Asymptotic analysis serves to identify the expressions for key quantities of interest, such as the (nonlinear) overall compliance, the sites and the magnitude of the maximum tensile stress, etc., in a scale-separated manner. Machine learning method is employed to embody those implicit interrelationships that are confirmed with asymptotic analysis. A number of simulation examples will be presented to show the balanced accuracy and efficiency of the proposed method. The presentation concludes with mathematical analogy to generalise the method used for analysing the behaviour of other multiscale systems.

Advances in numerical methods for solution of PDEs
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

A FAST PARALLEL SOLVING METHOD FOR THERMAL CONDUCTION-POISSON EQUATIONS BASED ON FAST FOURIER TRANSFORM

Jiang Zichao[*1], Huang Bohua[1], Wang Zhuolin[1] and Yao Qinghe[1]*

[1]*Sun Yat-sen University*

ABSTRACT

In the field of incompressible fluid dynamics and numerical heat transfer, the solution of Poisson and thermal conduction equations is usually one of the computational bottlenecks. To address this issue, this study introduces an innovative solution algorithm based on Fast Fourier Transform (FFT). The core of this algorithm is a FFT-based approach coupled with a variable reordering strategy, which transforms the global Poisson and thermal conduction equations into a series of sub-equations with a uniform structure. This enables compatibility with parallel computing architectures and significantly reduces computational complexity. Furthermore, the study has developed transformation algorithms suitable for Dirichlet, Neumann, and periodic boundary conditions. Numerical results indicate that our proposed method, when dealing with three-dimensional problems on a million-grid scale, surpasses traditional iterative methods by achieving more than a hundredfold acceleration. Additionally, the algorithm has been employed for direct numerical simulations of complex incompressible fluid and heat transfer problems, including vortex ring interactions, demonstrating its extensive applicability and high efficiency in practical scenarios.

TRANSIENT RESPONSE OF MAGNETO-RHEOLOGICAL FLUIDS IN HIGH SHEAR RATE REGIME

Sanket Chougale[1] *and Andreas Zilian**[1]

[1]*University of Luxembourg*

ABSTRACT

Magnetic field-responsive fluids are functional materials whose rheological properties can be controlled by an external magnetic field. The magneto-rheological (MR) fluid consists of magnetically soft (magnetizable) micron-sized particles suspended in a low-viscosity base fluid. Without an external magnetic field, MR fluids behave as a Newtonian fluid. On the other hand, the applied magnetic field introduces a rapid and reversible transition of an MR fluid from a free-flowing state to a solid-like behavior.
Understanding the transient characteristics of MR fluids, particularly the hydrodynamic response time of the fluid, is integral to the design of MR dampers. However, there is a scarcity of studies in the literature examining the hydrodynamic response time of magnetorheological fluids (MRFs) and their correlation with fluid properties. The response time of MRFs depends on several factors, such as the magnitude of the applied magnetic field, the dimensions of an MR valve, or the corresponding shear rates of MRFs. Thus, in this work, we investigate the transient behavior of MR fluid for a wide range (very low to high) of shear rates based on advanced constitutive relations for continuum-based fluid models.
Computational fluid dynamics (CFD) analysis has been carried out, and the results indicate that the higher the Bingham number, the lower the hydrodynamic response time of MRF. However, this only applies to low to moderate shear rate regimes, as recently reported in the literature [1, 2]. In the high shear rate regime, for the first time, we report that the response of MR fluid becomes much faster below a critical Bingham number. The observed phenomenon can be described by considering the notion of dwell time [2]. When the dwell time decreases significantly, especially falling below the response time under conditions of high shear rates, the MRF doesn't exhibit resistance to flow as expected for an applied magnetic field but rather only partial resistance. Our analysis implies that one must consider the effect of the dwell time on the response of MR fluid while designing an MR damper dealing with high velocities.

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Modeling and simulation of coupled processes in geological media
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

DEEP LEARNING ASSISTED MONITORING INVERSION MODEL FOR GEOLOGIC CARBON SEQUESTRATION

Jonathan Zingaro[*1], Robert Gracie[1] and Yuri Leonenko[1]*

[1]University of Waterloo

ABSTRACT

Geophysical monitoring is an important risk mitigation strategy used to assess the integrity of the subsurface during Carbon Sequestration injection and storage operations. There is a desire to assimilate various sparse geophysical measurements to achieve detailed and high-resolution monitoring of reservoirs. Traditional optimization and stochastic-based methods have been recognized as severely ill-posed and extremely computationally intensive, where real-time simulations are not possible. This work presents a robust deep learning-based inversion approach to model the time-dependent nature of predicting the saturation and pressure fields in the subsurface during CO2 injection and storage operations. This work employs a state-of-the-art, transformer-based deep learning architecture. This architecture utilizes the self-attention mechanism, which effectively learns the long-term dependencies of sequential data without the computational inefficiencies of recurrent hidden layers in Recurrent Neural Networks (RNNs) architectures. The training regime is generated through several high-fidelity simulations using a Finite Element-based quasi-3D vertically averaged multiphase flow simulation combined with a surface uplift geomechanical elasticity model. Multi-Gaussian porosity and permeability fields, varying injection schedules, and heterogeneity in the reservoir characterize the training regime. The performance of the proposed deep learning-assisted inversion model is demonstrated through a problem with highly heterogeneous subsurface permeability and porosity fields. The results show that the transformer-based architecture can accurately and computationally efficiently capture the long-term behaviour for high-dimensional inputs and outputs of nonlinear dynamical systems through the self-attention mechanism.

Keywords: Geomechanics, Inverse problem, Deep learning, Transformer, Monitoring, Carbon sequestration

Modeling and simulation for additive manufacturing
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

MULTIPHYSICS MODELING OF PROCESS–STRUCTURE–PROPERTY RELATIONSHIPS IN METAL 3D PRINTING

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[1]*University of New South Wales*

ABSTRACT

Enhancing properties of additively manufactured materials requires a comprehensive understanding of AM process-(micro)structure-property (PSP) relationships, which is currently limited. This calls for the development of tools that facilitate deepening this understanding and will support efficient materials engineering for AM.
In response, we have developed the computational suite of robust multi-physics models to support AM PSP research by enhancing the prediction capabilities in this space. This includes melt-pool-scale thermal simulations of metal AM, using the finite difference method, cellular automata simulations to describe the microstructure evolution during printing [1], micromechanical crystal-plasticity-based simulations with finite elements describe the mechanical behaviour of additively manufactured materials as well as the analytical approach to quickly estimate elastic properties of larger volumes [2]. The models have been validated experimentally.
This presentation covers the results of PSP modelling for alloys fabricated by laser powder bed fusion (mostly) and touches upon direct energy deposition. Effects of some process parameters on the microstructure and mechanical behaviour of AM metallic materials are analysed. High performance computing process-structure simulations are discussed. The integrative computational approach not only advances our understanding of AM but also enhances our ability to predict and control the properties of manufactured materials, addressing key barriers to the broader application of AM technologies.

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Numerical methods, mathematical modeling and analysis in material science
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

EFFECT OF THE CAPILLARY FORCE ON THE REPOSE ANGLE OF GRANULAR MATERIALS

Wang Ziye[*1] and Tan Yong*[1]

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ABSTRACT

The angle of repose does affect the behavior of granular materials and has a wide range of applications. The addition of a small amount of liquid can dramatically change the properties of granular media, leading to an increase in the repose angle. This change is mainly attributed to the capillary force resulting from the liquid bridge when the small amount of water was introduced. The capillary force as an attractive force increases the interaction between particles and becomes a dominant factor affecting the angle of repose because it is usually stronger than gravity. In this paper, a new discrete element method (DEM) model was developed in which the capillary force was calculated by the liquid bridge model based on "toroidal approximation"[1]. The developed DEM model linked the microscopic liquid bridge volume to the macroscopic water content and it also considered the effect of liquid bridge breakage and formation on capillary force. The numerical model was first validated by comparing the experimental and numerical results. Then, the effects of surface tension, volume of the liquid bridge, and the contact angle are studied numerically. Finally, the empirical equation between water content and angle of repose is given under the present simulation conditions. This work will provide a deep understanding for the effect of capillary on the angle of repose.

Keywords: repose angle; capillary force; liquid bridge model; DEM simulation

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Mathematical modeling and simulation for social, environmental, and disaster prevention issues
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

STRUCTURE AND NUMERICAL SOLUTION OF A THERMAL PROBLEM WITH IMPOSED INTERNAL CONDITIONS

Sergio Zlotnik[*12], Mariano Tomás Fernández[12] and Pedro Diez[1]*

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ABSTRACT

Undestanding the current state of Earth requires the knowledge of the location of several interfaces. One the the main ones is the Lithosphere-Asthenosphere Boundary (LAB). This is done via multibservable inversion schemes. One of the key fields to determine is the temperature. It affects almost all the other physical quantities involved (e.g. densities, viscosities, wave propagation velocities, among others).
The LAB affects most of the processes and properties in the Earth structure. Determining its location is one of the goals the inversions. The LAB is usually defined as an isotherm.
The need of determining the thermal field in accordance with a given LAB location leads to a mathematical problem with imposed interior conditions. In particular, the isotherm defining the LAB has to be located in the position tested by the inverse solver.
Here we analyze the mathematical structure of a thermal problem with known interior conditions and then propose several numerical procedures to solve it. The proposed methods are tailored to the geophysical case and are based on the certainty of the different boundary conditions that are imposed in the model. Moreover, because this thermal solver is expected to be used many times within an inverse scheme, we want the numerical mesh to be fixed. The LAB, therefore, will not fit the mesh.

Modeling and inverse design of architected materials
July 21-26, 2024, Vancouver Convention Centre, Vancouver, British Columbia, Canada

TOWARDS ZERO-POWER SPEECH RECOGNITION: IMPLEMENTING MACHINE-LEARNING MODELS IN MECHANICAL STRUCTURES

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ABSTRACT

Elastic metamaterials, with their minimal energy dissipation during vibration, present a promising solution for ultra-low-power applications like the Internet of Things. However, taking advantage of these unique properties to do information processing tasks (for example, speech recognition for command detection) is a challenging computational design problem. In this talk, I will describe our results regarding the development of a mechanical resonator network capable of performing speech recognition. The design approach we have chosen is based on a proven speech recognition architecture. In our model, a support vector machine (SVM) operates on a set of features obtained from calculating the energy content across various frequency bands. We employ a multi-step procedure to transfer this model into the mechanical domain. First, the model is mapped to a lumped, nonlinear mass-spring model, which is then translated to a device geometry in a second step. A comparison of the mass-spring model to standard benchmarks for few-word classification reveals that, in addition to delivering comparable accuracies to electronic speech recognition implementations, it reduces energy consumption by multiple orders of magnitude.
The mass-spring model is optimized by using adjoint back-propagation in time and then mapped to a geometry by implementing each degree of freedom using structural modes from drums, strings, and cantilever resonators. We subject these components to finite element simulations, optimizing them to exhibit the required dynamic characteristics as designed in the abstract model. Creating neural networks involves thousands of components, which makes simulations and optimizations time-consuming. To overcome this challenge, we use sub-structuring techniques to reduce the size of mass, stiffness, and damping matrices, replacing some of the degrees of freedom in the FEM model with normal modes. We then apply adjoint-based optimization methods to identify the geometric parameters that are most conducive to word classification accuracy.

STABILITY AND CRACK NUCLEATION IN VARIATIONAL PHASE-FIELD MODELS OF FRACTURE: EFFECT OF LENGTH-SCALES AND MULTI-AXIALITY

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ABSTRACT

Phase-field model for brittle fracture is widely used due to its ability to reproduce complex crack patterns, without ad hoc criteria, and to deal with the behavior of crack formation under tensile loading. However, crack nucleation under multi-axial stress states in phase-field model remains a subject of discussion with several unresolved issues. Among these, we identify the inability to flexibly set the crack nucleation criterion under multi-axial stress states and the difficulty in modeling crack nucleation in materials close to the incompressibility limit. In this contribution, we focus on the evolution of a special class of phase-field models with linear softening [1] in order to overcome the aforementioned limitations. These models provide increased flexibility in adjusting the crack nucleation criterion by allowing the use of different softening laws on the volumetric and deviatoric components of the strain energy density. However, the choice of the softening law has an impact on crack nucleation and reveals the length-scales which influence the stability of the solution. Therefore, we conduct a theoretical and numerical stability analysis, inspired by the work of [2-3]. Through this stability analysis, we establish the limitations of this model in describing crack nucleation in nearly inextensible bars (the 1D version of almost incompressible materials) and under multi-axial stress states and we explain the connection between fracture nucleation and the competition between stored elastic energy and fracture energy.

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Numerical modelling of composite materials and structures
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A LAYERED SOLID FINITE ELEMENT FORMULATION WITH INTERLAMINAR ENHANCED DISPLACEMENTS FOR THE MODELING OF LAMINATED COMPOSITE STRUCTURES

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ABSTRACT

Laminated composite materials are widely used in many engineering industries today ranging from aerospace applications, fuel storage pressure vessels, automotives, etc. Their increased usage has motivated the need for improved finite element modeling capabilities to aid in the design and assessment of composite structures. Current modeling approaches for layered composite materials range from homogenized material models in the form of an effective continuum-level anisotropic material model, to finely discretized mutli-scale models wherein each of the individual material plies are discretized at the micro/mesoscale level. Both approaches are subject to different limitations: homogenized material models do not explicitly consider the behavior of individual plies, whereas multi-scale modeling approaches may incur prohibitively high computational costs.

To address the limitations of both ranges of modeling granularity, an 8-node layered solid hexahedral finite element is formulated with the aim of striking an appropriate balance between efficiency and fidelity. The element may be discretized into an arbitrary number of material layers and employs a reduced in-plane integration scheme in each layer for computational efficiency along with supplementary physical stabilization based upon the stabilization scheme of Puso [1]. While many existing solid shell formulations similarly adopt physical stabilization with reduced in-plane integration, the novelty of the proposed approach lies in its use of layerwise enhancements to accurately represent the stabilizing material stiffness contributions from each layer and eliminate various forms of locking phenomena. Additionally, the chosen framework supports the inclusion of interlaminar enhanced displacements to enforce continuity of interlaminar tractions and further reduce locking behavior in general layered composites. The element has been implemented in the ParaDyn finite clement code [2], and its efficacy for modeling laminated composite structures has been demonstrated on a variety of verification problems.

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SINDY-RL: INTERPRETABLE AND EFFICIENT REINFORCEMENT LEARNING

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ABSTRACT

Deep Reinforcement Learning (DRL) has shown significant promise for uncovering sophisticated control policies that interact in environments with complicated dynamics, such as stabilizing the magnetohydrodynamics of a tokamak reactor and minimizing the drag force exerted on an object in a fluid flow. However, these algorithms require many training examples and can become prohibitively expensive for many applications. In addition, the reliance on deep neural networks results in an uninterpretable, black-box policy that may be too computationally challenging to use with certain embedded systems. Recent advances in sparse dictionary learning, such as the Sparse Identification of Nonlinear Dynamics (SINDy), have shown to be a promising method for creating efficient and interpretable data-driven models in the low-data regime. In this work, we extend ideas from the SINDy literature to introduce a unifying framework for combining sparse dictionary learning and DRL to create efficient, interpretable, and trustworthy representations of the dynamics model, reward function, and control policy. We demonstrate the effectiveness of our approaches on benchmark control environments and challenging fluids problems, achieving comparable performance to state-of-the-art DRL algorithms using significantly fewer interactions in the environment and an interpretable control policy orders of magnitude smaller than a deep neural network policy.

Advanced numerical methods for the modeling and optimization of coupled dynamical systems
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MATHEMATICAL AND EXPERIMENTAL MODELING OF A STOCKBRIDGE DAMPER USED TO SUPPRESS AEOLIAN VIBRATION OF TRANSMISSION LINE CONDUCTORS

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ABSTRACT

The Stockbridge vibration damper is significantly used in overhead transmission lines to mitigate Aeolian vibration. Aeolian vibrations refer to the oscillations of conductor cables within the frequency range of 3–150 Hz. The effectiveness of the Stockbridge damper is characterized by the number of resonant frequencies. Unlike the basic Stockbridge damper, which features only two resonant frequencies, the asymmetric Stockbridge damper demonstrates the capability to exhibit up to four resonant frequencies. Previous numerical simulations and parametric studies have established a correlation between the increase in natural frequencies and alterations in the counterweight's geometry. In this paper experiments have been conducted on the modified asymmetric damper and an analytical model has been developed. This paper confirms the research that was done by Vaja, Barry, and Tanbour.

Keywords-Stockbridge damper, Analytical model, Aeolian vibration

Multiscale computational and data-driven approach of advanced materials and structures
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COARSE-GRAINED MOLECULAR DYNAMICS SIMULATION OF HYDROGEL MICROSTRUCTURES

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ABSTRACT

Hydrogels are composed of cross-linked polymer network wrapped with a large amount of water. It has large deformation, strong toughness, and are currently attracted considerable attention owing to their unique mechanical properties. The microstructure and dissipation mechanism of polymer networks in hydrogels are the basis for their desired properties. Hence, we proposed a practical and efficient data-inspired method for coarse-grained molecular dynamics model with greatly simulation efficiency compared to all-atom molecular dynamics simulation. Furthermore, the correlation between copolymer ion gel components and macroscopic properties was established to explore the relationship between microstructure and tensile properties. We observed and analyzed the viscoelasticity by the coarse-grained hydrogel models with extensive dissipation mechanisms and by uniaxial elongation simulations. The coarse-grained molecular dynamic simulation of hydrogels successfully described the microstructure of hydrogels, explored the strength mechanism of hydrogels, reduced the difficulty of constructing multi-scale models, and expanded the intelligent application of hydrogels.

REDUCED-ORDER MODELING OF UNSTEADY CONVECTION-DOMINATED PROBLEMS BY IMPLICIT FEATURE TRACKING

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ABSTRACT

For convection-dominated problems, failure to build accurate reduced-order models (ROMs) has been mainly attributed to the slowly decaying Kolmogorov n-width of linear subspace approximations. This is also sometimes referred to as Kolmogorov barrier because the error slowly decaying with the dimension of the reduced space limits the achievable accuracy of ROMs in practice and requires a substantial amount of training data, which can be infeasible to collect offline. In this work we propose an arbitrary Lagrangian-Eulerian approach that improves the accuracy of time-dependent conservation laws by implicitly aligning the solutions in the computational domain. The mapping between the fixed (computational) geometry and the physical space are given by Lagrange interpolation functions computed by solving an optimization problem that minimizes the residual. Afterwards, the resulting state solutions and mappings obtained are used in the following to generate projection-based ROMs with improved predictive capabilities. The approach is tested and validated on different convection-dominated problems.

IMMERSED TECHNIQUES FOR SIMULATING FLOW AND TRANSPORT IN FRACTURED POROUS MEDIA

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ABSTRACT

The ever-increasing computational power of modern supercomputers enables the numerical simulation of complex and coupled large-scale multiphysics problems, e.g., arising from fluid-structure interaction, or geometrically complex interactions, e.g., in contact mechanics. Common to these coupled and complex problems is the need to transfer data or information between the different models, meshes, or approximation spaces. The transfer of discrete fields, such as stresses, pressure, displacements, or velocities, might be required along surfaces or within volumes. Variational transfer techniques might also play an essential role at the level of the discretization, e.g., within non-conforming domain decomposition or mortar methods for the transfer along surfaces, or on the level of the solution method, e.g., within multigrid or multi-level methods for the transfer between different volume meshes. This talk introduces our parallel variational transfer technique and its application to flow and transport in fractured porous media.

Modeling friction and wear
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AN EXTENSIVE THERMAL AND STRESS ANALYSIS OF RAILWAY WHEEL-RAIL CONTACT DURING HEAVY BRAKING WITH DISC BRAKE

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ABSTRACT

Railways have become increasingly popular as safe and less polluting forms of traffic both in short and long distances and in passenger and freight transports. More and more new safety features, like the anti-slip WSP - Wheel Slide Protection System, are in service with their development. Still, these developments sometimes cause undesired effects, such as micro-thermal wheel tread cracks [1].

During intensive wheel-braking of railway vehicles equipped with disk brakes, the wheel slides on the rail. While the macroscopic sliding speed is restricted, it is not excluded by the WSP. There is a remarkable heat generation through the frictional sliding process between the parts in contact. This heat may cause micro-cracks on and under the wheel tread.
In earlier publications [2] [3], the modeling method was presented using ANSYS, which provided the opportunity to examine and understand the background of this phenomenon using numerical calculations. Furthermore, using an extended FE model, the effect of the different operation conditions (movement speed, different coefficient of friction, etc.) and the coupled effect of the micro-cracks and the subsurface fatigue cracks could be observed [3].

In the current state of the research, the modeling method was adopted for different vehicles (contact geometries, loading conditions) and operating conditions (such as winter or summer using different frictional environments). These extended analyses provided the opportunity to create widespread trends that show the possible micro-cracking in the function of several operating factors (different frictional environments). The results of these coupled transient thermal and elastic-plastic frictional contact and further crack FE simulations provide the opportunity to understand the limits of these WSP systems. It can help minimize the failures of the wheels and the rail using an appropriate setup of this safety feature.

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Contact and interface mechanics: Modeling and computation
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FLUID-STRUCTURE INTERACTION SIMULATIONS OF NUCLEAR POWER PLANT STEAM GENERATOR TUBES INVOLVING CONTACT

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ABSTRACT

In the evolving landscape of nuclear energy, ensuring the safety and efficiency of nuclear reactors remains paramount, particularly with the increasing demands for energy and a concurrent rise in global temperatures. A significant aspect of nuclear safety and efficiency involves maintaining the structural integrity of the nuclear steam supply system (NSSS). In particular, key NSSS components such as fuel assemblies (FA) or steam generator (SG) tubes are susceptible to flow-induced vibrations (FIV) resulting from the turbulent flow of the coolant. FIV can instigate severe repercussions, including structural damage such as fatigue and wear, caused by the repetitive oscillatory motion of these components and the rubbing or sliding contact between them and surrounding parts. In particular, grid-to-rod-fretting wear (GTRFW) resulting from such vibrations is the cause of 58% of fuel failures in pressurized water reactors [1].

Despite the attention FIV of FA and SG tubes has garnered since the 1950s, conventional semi-empirical methods offer limited predictive accuracy and do not facilitate extrapolations for multi-rod scenarios effectively, while experiments are complex and complicated to perform, not in the last place due to the harsh environment. With the increased computational power available today, numerical methods are more frequently used to estimate the tubes' displacements. The used methods and models have increased in complexity in time, and are generally quite well able to predict the vibration frequency and, to a lesser extent, the amplitude of displacement of the moving tubes. However, they seldomly involve contact between neighboring tubes or between tubes and the fixed surroundings, while this contact causes the wear leading to structural degradation and eventual failure of the component. Such contact also has a significant effect on the vibrational frequency [2].

The current presentation shows initial work done on performing Fluid-Structure Interaction simulations involving contact, using the commercial software Simcenter STAR-CCM+. The case under consideration is that of a cylinder subjected to cross-flow, representative of the U-bend area of a SG tube, the area of most concern for FIV of SG tubes in nuclear power plants. Amongst others, the influence of the inflow velocity and material properties are studied on the observed vibration behavior and resulting contact.

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