PURSUING TRUSTWORTHY MACHINE LEARNING FOR MULTISCALE META-MODELING OF MATERIALS

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ABSTRACT

While there are many works dedicated to showcase the promise of machine learning for scientific problems, this talk attempts to demonstrate both the advantages and drawbacks of a collection of state-of-the-art machine learning techniques commonly used to characterize, predict, and design mechanical properties for mechanics of solids and structures. We first discuss the issue of lack of interpertability of machine learning models that often leads to distrust of end-users in engineering mechanics domains. In particular, we introduce two techniques that combines the strength of the expressivity of neural networks and the interpretability of mathematical models to create a material models that can easily be implemented across conventional platforms such as UMAT, one based on knowledge graph [1] and another one based on neural neural feature space [2]. We then explore the relationships between data availability and dimensionality of material models [4]. In particular, we will discuss how deep reinforcement learning [1] and active learning [3] enable more efficient long-term planning for experiments. We will also explore how to balance the need for exploitation and exploration as well as how well known physics principles such as material symmetry and thermodynamics constraints may enable both more efficiency used of data. Finally, we will highlight a recent work that enables multi-fidelity phase field models in which a diverse collections of deep learning and multiscale models, each of different speed and forward prediction capacity, are used to predict the same materials responses in a space-time continuum domain. By introducing a driving force that estimate the infidelities of different models, the optimal ensembles of constitutive models are formulated to predict various types of material failures for solid undergoing irreversible deformation.

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