Learning Nonlocal Constitutive Laws for Material Fracture Modeling

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Workshop on Experimental and Computational Fracture Mechanics

March 4, 2024

Motivation and Background

Goal: data-driven prediction of material responses

- Prediction and monitoring of complex material responses from experimental measurements are ubiquitous in applications from different fields, such as mechanical engineering, biomedical engineering, civil engineering, etc.

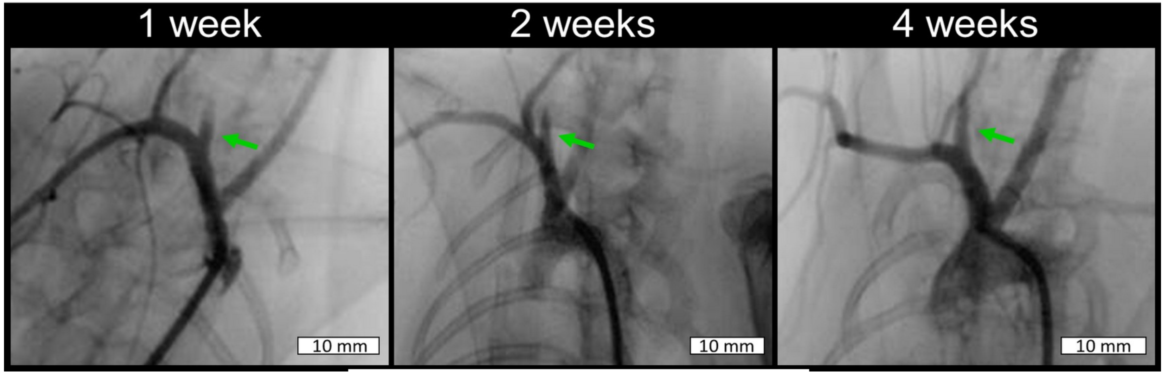
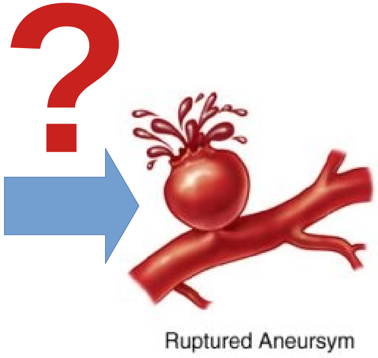
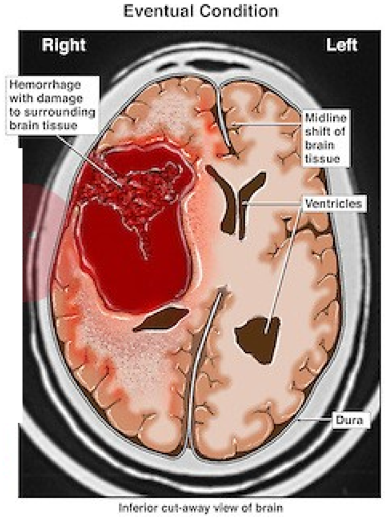


Image by Chung-Hao Lee





Example 1: monitor aneurysm status and predict the possible hemorrhagic stroke.

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UAV

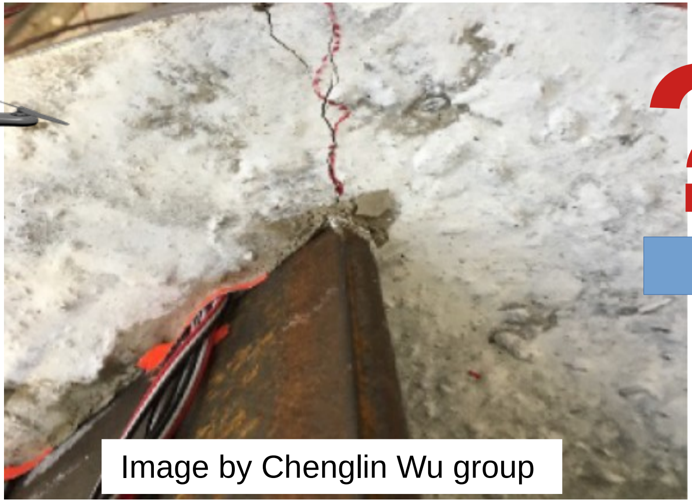
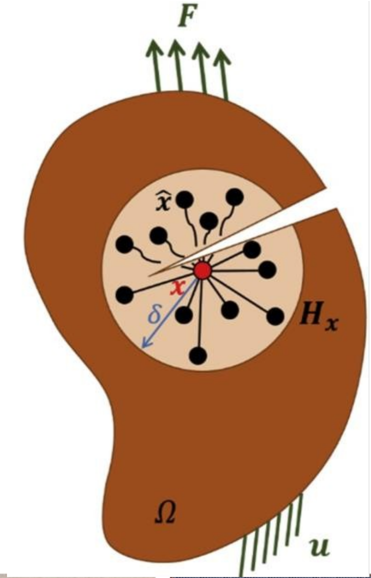


Image by Chenglin Wu group

Image by Francesco Pugliese

Example 2: monitor crack propagation and corrosion to predict the bridge serving life.

What is (spatially) nonlocal model?



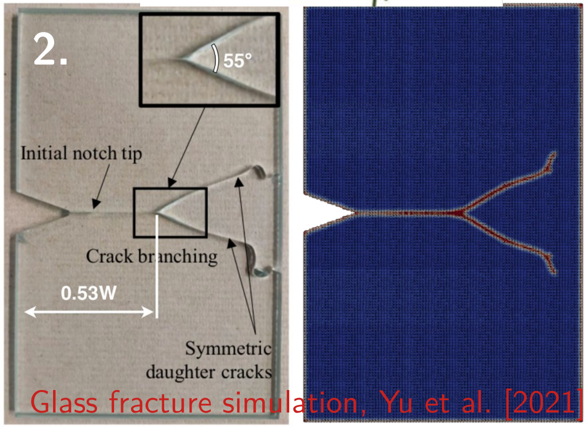
Basic concepts:

- The state of a system at any point depends on the state in a **neighborhood** of points
- Interactions can occur **at distance, without contact**
- Solutions can be irregular: non-differentiable, singular, discontinuous

Facts:

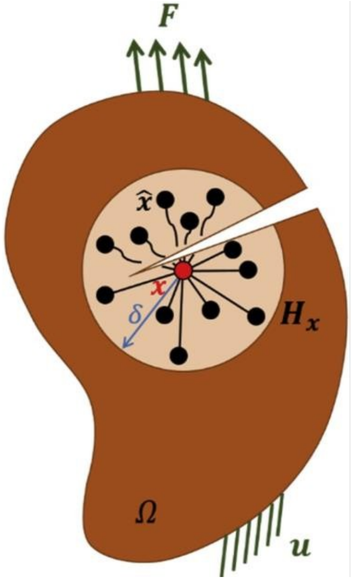
These models can capture effects that traditional PDEs **hard to capture**

1) Multiscale behavior (*nonlocal as an upscaled/homogenized model*)
2) Discontinuities such as cracks and fractures
3) Anomalous behavior such as superdiffusion and subdiffusion *(fractional operators)*



Glass fracture simulation, Yu et al. [2021]

What is (spatially) nonlocal model?



Basic concepts:

- The state of a system at any point depends on the state in a **neighborhood** of points
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- Solutions can be irregular: non-differentiable, singular, discontinuous

A general nonlocal mechanical (peridynamics) model:

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \int_{B_\delta(\mathbf{x})} \boxed{\mathbf{b}(\mathbf{y},\mathbf{x},\mathbf{u},t)\ d\mathbf{y}} + \mathbf{f}(\mathbf{x},t)$$

The integrant depends on material properties, microstructure, etc.

Learn the integrants from data pairs $\{\mathbf{u}_i(\mathbf{x},t),\mathbf{f}_i(\mathbf{x},t)\}_{i=1}^{N}$

S. A. Silling, Reformulation of elasticity theory for discontinuities and long-range forces, Journal of the Mechanics and Physics of Solids 48 (1) (2000) 175–209.

Proposed: Nonlocal Constitutive Law

- **Goal:** identify a nonlocal integrant in $\mathcal{G}[\mathbf{u}](\mathbf{x},t) := \int_{B_\delta(\mathbf{x})} \mathbf{b}(\mathbf{y},\mathbf{x},\mathbf{u},t)\, d\mathbf{y}$

s.t.,
$$\begin{cases} \rho\ddot{\mathbf{u}} = \mathcal{G}_{[k,\underline{\mathbf{T}},d]}\mathbf{u} + \mathbf{f} & \text{in } \Omega \\ \mathbf{u} = \mathbf{u}_{bc} & \text{on the nonlocal boundary } \Omega_\delta \end{cases}$$

1) **Collect measurements** of function pairs: $\mathcal{D} = \{\mathbf{u}_j(\mathbf{x},t), \mathbf{f}_j(\mathbf{x},t)\}_{j=1}^N$

Training set: measurements or high fidelity simulations

2) **Approximate the integrant** with a parameterization:

Homogenized model[1] $\mathbf{b}(\mathbf{y},\mathbf{x},\mathbf{u},t) := k(|\mathbf{x}-\mathbf{y}|)d(\mathbf{x},\mathbf{y},\mathbf{u},t)(\mathbf{u}(\mathbf{y},t)-\mathbf{u}(\mathbf{x},t))$

Generic model[2] $\mathbf{b}(\mathbf{y},\mathbf{x},\mathbf{u},t) := \underline{\mathbf{T}}(\mathbf{x},\mathbf{y},\mathbf{u})d(\mathbf{x},\mathbf{y},\mathbf{u},t)$

Outcomes:
1. material-specific kernel function k, force state $\underline{\mathrm{T}}$, and damage field d.
2. the surrogate model
$$\mathcal{G}_{[k,\underline{\mathbf{T}}]}\mathbf{u} = \mathbf{f}$$
for downstream tasks.

3) **Minimize the residual**

$$\mathcal{E}_\lambda(k,\underline{\mathbf{T}},d) = \frac{1}{N}\sum_{j=1}^{N} \|\mathcal{G}_{[k,\underline{\mathbf{T}},d]}[\mathbf{u}_j] + \mathbf{f}_j - \rho\ddot{\mathbf{u}}_j\|_{L^2}^2 + \lambda\mathcal{R}(k,\underline{\mathbf{T}},d)$$

[1]H. You, Y. Yu, N. Trask, M. Gulian, M. D'Elia, "Data-driven learning of nonlocal physics from high-fidelity synthetic data", CMAME, Volume 374, 113553, 2021.
[2]S. Jafarzadeh, N. Liu, S. Silling, Z. Zhang, Y. Yu*. (2024). "Peridynamic Neural Operators: A Data-Driven Nonlocal Constitutive Model for Complex Material Responses".

Nonlocal Operator vs PDE Learning

- Nonlocal models replaces the derivatives in PDEs with integral operators.
- Solutions can be irregular: non-differentiable, singular, discontinuous.

Pros:

1) Nonlocal models are a broader family of equations, and therefore can capture effects that traditional PDEs **hard to capture**.
2) The material heterogeneity can also be embedded in the kernel.
3) Many **mathematical tools** of PDEs have analogs in nonlocal models, making the well-posedness analysis possible.

Cons:

1) The boundary condition of nonlocal models should be described in a region, not in just a layer.

   (The boundary region is provided by data)
2) The assembly and solution of nonlocal problems are generally more expensive than with classical PDEs.

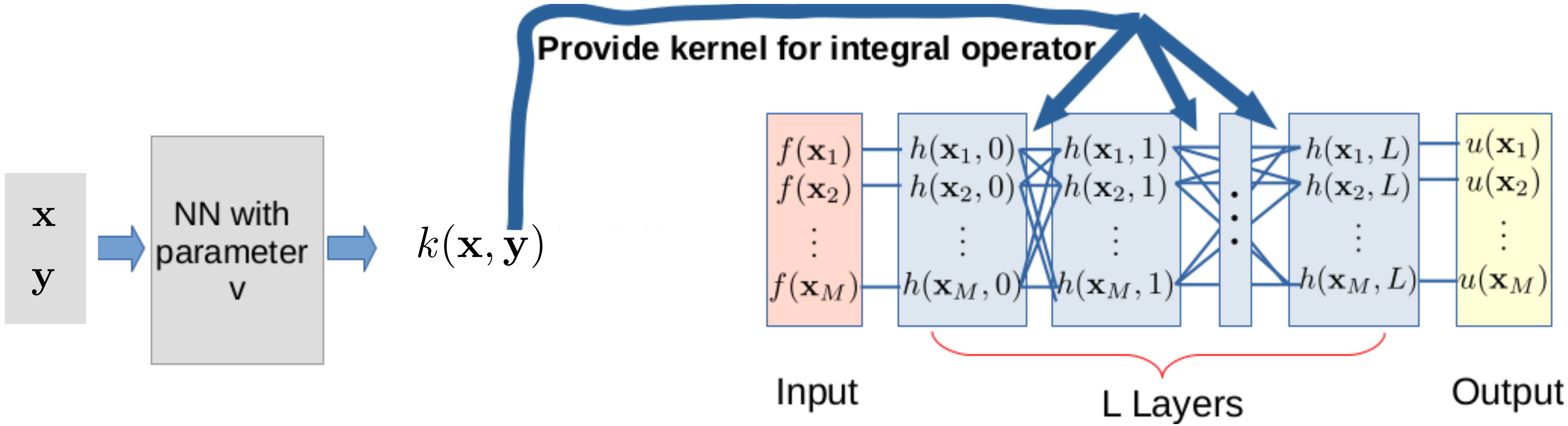
   (Evaluation of Integrals can be accelerated using GPUs and sometimes FFTs)

Nonlocal Operator vs Neural Network

- In contrast to classical neural networks which provides a vector-to-vector mapping, nonlocal operator provides a data-driven **surrogate mapping between two function spaces**.

Classical NN: $h_i^{l+1} = \sigma\left(\sum_{j=1}^{N} W_{ij}^l h_j^l\right)$

Nonlocal Operator: $h^{l+1}(x_i) = \sigma\left(\int k(x_i, y) h^l(y) dy\right) \approx \sigma\left(\Delta x \sum_{j=1}^{N} k(x_i, x_j) h^l(x_j)\right)$



Nonlocal Operators: different resolution has invariant parameters

[1]Z. Li, N. Kovachki, K. Azizzadenesheli, B. Liu, K. Bhattacharya, A. Stuart, A. Anandkumar, Neural operator: Graph kernel network for partial differential equations, arXiv preprint arXiv:2003.03485.

Part I
Learning Nonlocal Kernel for Homogenized Models

[1] H. You, Y. Yu*, S. Silling, M. D'Elia, "A data-driven peridynamic continuum model for upscaling molecular dynamics". CMAME, 2022.
[2] F. Lu, Q. An, Y. Yu*, "Nonparametric learning of kernels in nonlocal operators". JPER,2023.
[3] H. You, Y. Yu, S. Silling, M. D'Elia, "Data-driven learning of nonlocal models: from high-fidelity simulations to constitutive laws". AAAI Spring Symposium: MLPS, 2021
[4] H. You, Y. Yu, N. Trask, M. Gulian, M. D'Elia, "Data-driven learning of nonlocal physics from high-fidelity synthetic data", CMAME, 2021.
[5] H. You, L. Zhang, Y. Yu, "A meta-learnt nonlocal operator regression approach for metamaterial modeling". MRS Communications, 2022.
[6] Fan Y., D'Elia M, Yu Y, Najm H., Silling S. "Bayesian Nonlocal Operator Regression (BNOR): A Data-Driven Learning Framework of Nonlocal Models with Uncertainty Quantification". Submitted, 2022

Homogenized Nonlocal Constitutive Law

- **Goal:** identify a nonlocal integrant in $\mathcal{G}[\mathbf{u}](\mathbf{x},t) := \int_{B_\delta(\mathbf{x})} \mathbf{b}(\mathbf{y},\mathbf{x},\mathbf{u},t)\, d\mathbf{y}$

s.t.,
$$\begin{cases} \rho\ddot{\mathbf{u}} = \mathcal{G}_{[k,d]}\mathbf{u} + \mathbf{f} & \text{in } \Omega \\ \mathbf{u} = \mathbf{u}_{bc} & \text{on the nonlocal boundary } \Omega_\delta \end{cases}$$

Training set: measurements or high fidelity simulations

1) **Collect measurements** of function pairs: $\mathcal{D} = \{\mathbf{u}_j(\mathbf{x},t), \mathbf{f}_j(\mathbf{x},t)\}_{j=1}^N$
2) **Approximate the integrant** with a parameterization:

Homogenized model[1] $\mathbf{b}(\mathbf{y},\mathbf{x},\mathbf{u},t) := k(|\mathbf{x}-\mathbf{y}|)d(\mathbf{x},\mathbf{y},\mathbf{u},t)(\mathbf{u}(\mathbf{y},t) - \mathbf{u}(\mathbf{x},t))$

$$k(|\mathbf{x}-\mathbf{y}|) = \sum_{m=1}^{M} \frac{c_m}{|\mathbf{x}-\mathbf{y}|^\alpha} \phi_m(|\mathbf{x}-\mathbf{y}|)$$

$$d(\mathbf{x},\mathbf{y},\mathbf{u},t) = \begin{cases} 0 & \text{if } S(\mathbf{x},\mathbf{y},\mathbf{u},\tau) > s_0 \text{ for some } \tau \le t \\ 1 & \text{else.} \end{cases}$$

3) **Minimize the residual**

$$\mathcal{E}_\lambda(k,d) = \frac{1}{N}\sum_{j=1}^{N} \|\mathcal{G}_{[k,d]}[\mathbf{u}_j] + \mathbf{f}_j - \rho\ddot{\mathbf{u}}_j\|_{L^2}^2 + \lambda\mathcal{R}(k,d)$$

Outcomes:
1. material-specific kernel function k, and damage criteria d.
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[1]H. You, Y. Yu, N. Trask, M. Gulian, M. D'Elia, "Data-driven learning of nonlocal physics from high-fidelity synthetic data", CMAME, Volume 374, 113553, 2021.
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Challenges:

1. Small data in damage regime
2. The residual is not differentiable with respect to s_0

Outcomes:
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1) **Collect measurements** of function pairs

without damage: $\mathcal{D} = \{\mathbf{u}_j(\mathbf{x},t), \mathbf{f}_j(\mathbf{x},t)\}_{j=1}^N$, and with damage: $\tilde{\mathcal{D}} = \{\tilde{\mathbf{u}}_j(\mathbf{x},t), \tilde{\mathbf{f}}_j(\mathbf{x},t)\}_{j=1}^{\tilde{N}}$.

Training set: measurements or high fidelity simulations

2) **Approximate the integrant** with a parameterization:

$$\mathbf{b}(\mathbf{y},\mathbf{x},\mathbf{u},t) := k(|\mathbf{x}-\mathbf{y}|)d(\mathbf{x},\mathbf{y},\mathbf{u},t)(\mathbf{u}(\mathbf{y},t) - \mathbf{u}(\mathbf{x},t))$$

3) **Step 1: Learn the kernel by minimizing the residual on D**

$$k(|\mathbf{x}-\mathbf{y}|) = \sum_{m=1}^{M} \frac{c_m}{|\mathbf{x}-\mathbf{y}|^\alpha}\phi_m(|\mathbf{x}-\mathbf{y}|)$$

$$\mathcal{E}_\lambda(k) = \frac{1}{N}\sum_{j=1}^{N} \|\mathcal{G}_{[k]}[\mathbf{u}_j] + \mathbf{f}_j - \rho\ddot{\mathbf{u}}_j\|_{L^2}^2 + \lambda\mathcal{R}(k)$$

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without damage: $\mathcal{D} = \{\mathbf{u}_j(\mathbf{x},t), \mathbf{f}_j(\mathbf{x},t)\}_{j=1}^{N}$, and with damage: $\tilde{\mathcal{D}} = \{\tilde{\mathbf{u}}_j(\mathbf{x},t), \tilde{\mathbf{f}}_j(\mathbf{x},t)\}_{j=1}^{\tilde{N}}$.

2) **Approximate the integrant** with a parameterization:

$$\mathbf{b}(\mathbf{y},\mathbf{x},\mathbf{u},t) := k(|\mathbf{x}-\mathbf{y}|)d(\mathbf{x},\mathbf{y},\mathbf{u},t)(\mathbf{u}(\mathbf{y},t) - \mathbf{u}(\mathbf{x},t))$$

3) **Step 2: Optimize a smoothed damage criteria on D**

$$d(\mathbf{x},\mathbf{y},\mathbf{u},t) = \frac{1}{2}\left(-tanh\left(\frac{\max_{\tau\le t} S(\mathbf{x},\mathbf{y},\mathbf{u},\tau) - s_0}{\eta}\right) + 1\right)$$

$$\mathcal{E}_\lambda(d) = \frac{1}{\tilde{N}} \sum_{j=1}^{N} \|\mathcal{G}_{[k^*,d]}[\tilde{\mathbf{u}}_j] + \tilde{\mathbf{f}}_j - \rho\ddot{\tilde{\mathbf{u}}}_j\|_{L^2}^2 + \lambda\mathcal{R}(d)$$

Training set: measurements or high fidelity simulations

Outcomes:
1. material-specific kernel function k, and damage criteria d.
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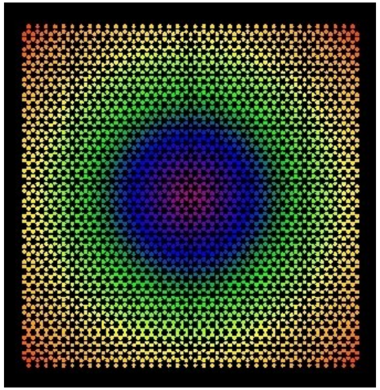
Homogenized NO: Coarse-grained MD model

- Given: a collection of samples of coarse-grained MD displacements and forcing $\{(\mathrm{u}_i, \mathbf{f}_i)\}_{i=1}^N$

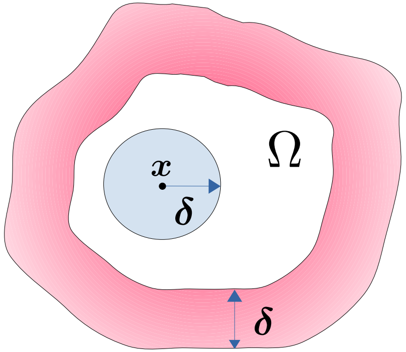


- Model: linearized peridynamic solid (LPS) model

$$\mathcal{L}_\delta \mathbf{u} := -\frac{C_\alpha}{m(\delta)} \int_{B_\delta(\mathbf{x})} (\lambda - \mu) K(|\mathbf{y}-\mathbf{x}|)(\mathbf{y}-\mathbf{x})(\theta(\mathbf{x}) + \theta(\mathbf{y}))\, d\mathbf{y}$$
$$- \frac{C_\beta}{m(\delta)} \int_{B_\delta(\mathbf{x})} \mu K(|\mathbf{y}-\mathbf{x}|) \frac{(\mathbf{y}-\mathbf{x}) \otimes (\mathbf{y}-\mathbf{x})}{|\mathbf{y}-\mathbf{x}|^2} (\mathbf{u}(\mathbf{y}) - \mathbf{u}(\mathbf{x}))\, d\mathbf{y} = \mathbf{f}(\mathbf{x}) \quad \mathbf{x} \in \Omega,$$
$$\theta(\mathbf{x}) := \frac{d}{m(\delta)} \int_{B_\delta(\mathbf{x})} K(|\mathbf{y}-\mathbf{x}|)(\mathbf{y}-\mathbf{x}) \cdot (\mathbf{u}(\mathbf{y}) - \mathbf{u}(\mathbf{x}))\, d\mathbf{y}, \quad \mathbf{x} \in \Omega,$$
$$\mathcal{B}_I \mathbf{u}(\mathbf{x}) = \mathbf{q}(\mathbf{x}) \quad \mathbf{x} \in \Omega_I.$$

where the kernel K is approximated by Bernstein polynomials:

$$\mathrm{K}(|\mathbf{y}-\mathbf{x}|) = \sum_{m=0}^{M} \frac{C_m}{\delta^{d+2-\alpha} |\mathbf{y}-\mathbf{x}|^\alpha} B_{m,M}\left(\left|\frac{\mathbf{y}-\mathbf{x}}{\delta}\right|\right) \text{ when } |\mathbf{y}-\mathbf{x}| < \delta$$

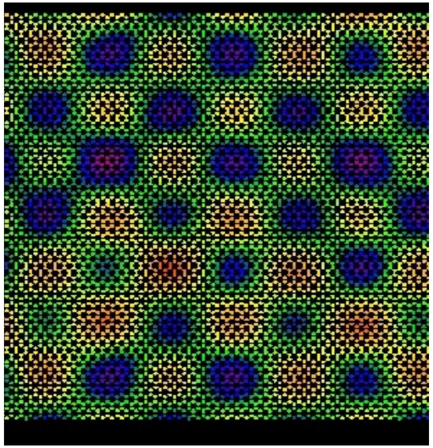


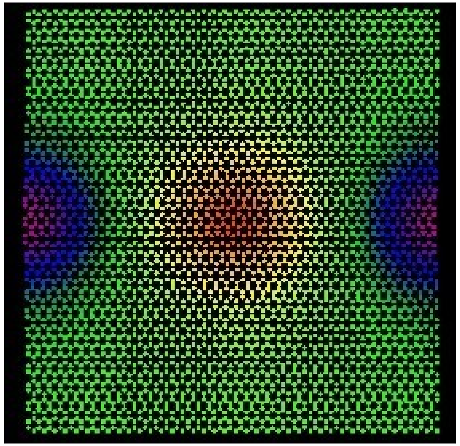
- Goal: approximate the kernel K(|y-x|), Youngs modulus E, Poisson ratio ν, and damaga criteria s_0.

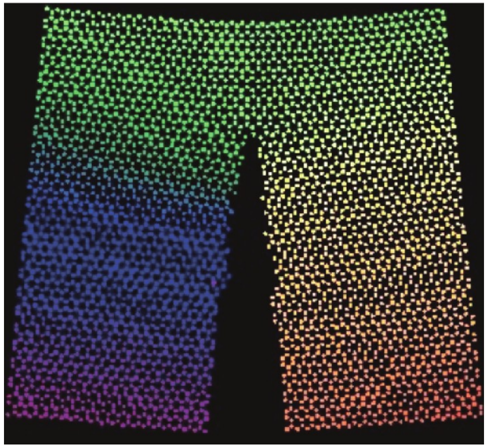
H. You, Y. Yu*, S. Silling, M. D'Elia, "A data-driven peridynamic continuum model for upscaling molecular dynamics". CMAME, 2022.

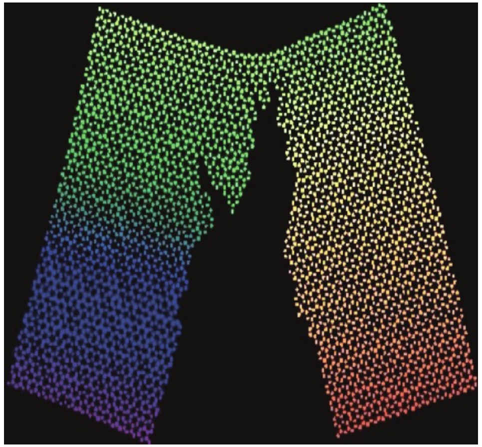
Homogenized NO: Coarse-grained MD model

- Data generation: perform MD modeling and coarse graining of a perfect graphene sheet at constant temperature (0 or 300K).









70 static training samples:
under loads with different frequencies

10 static validation samples:
under different point loads

1 dynamic training sample with damage:
under prescribed velocities on left and right edges

1 dynamic test sample with damage:
under a non-zero pulse force to open the slit

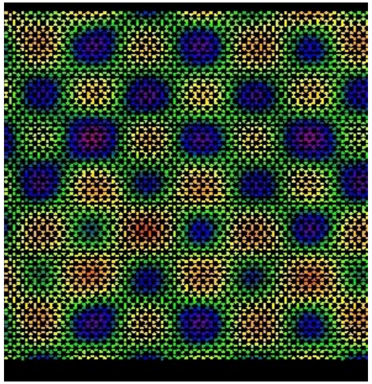
No damage training set D (70 static training samples and 10 static validation samples)

With damage training set D (1 dynamic training sample with damage)

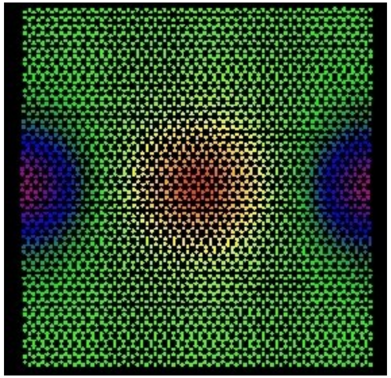
Coarse-grained MD model: No Damage

- Perform MD modeling and coarse graining of a perfect graphene sheet: Learn from square domains and test on circular domains.

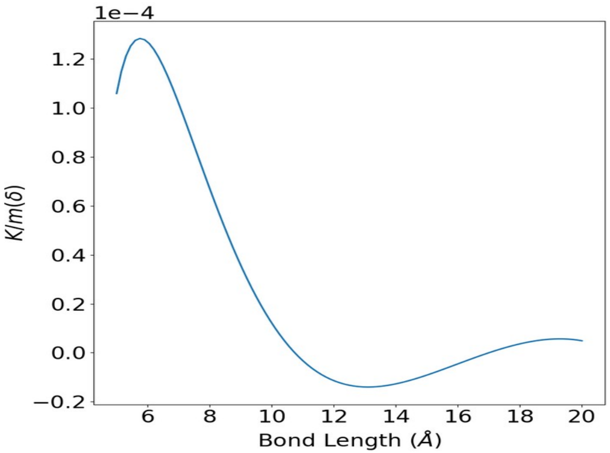
Training set	Young's modulus	Poisson ratio	α	Training Loss	Training error in u	Validation Loss	Validation error in u	Test error in u
0K	0.91 TPa	-0.43	2.8	9.81%	11.72%	13.28%	7.16%	**6.75%**
300K, Low	0.90 TPa	-0.42	2.6	9.82%	13.16%	18.08%	8.88%	**9.21%**



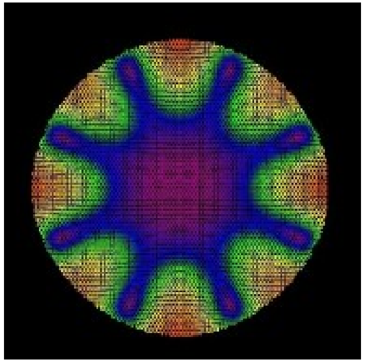
training



validation



learnt kernel



4 test samples: MD data

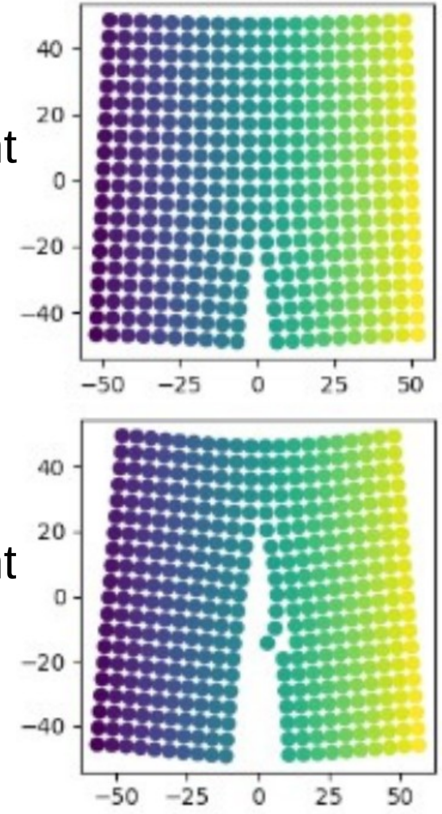
Coarse-grained MD model: With Fracture

- Learning damage criteria from one crack propagation case.

Training data (Δx=5)

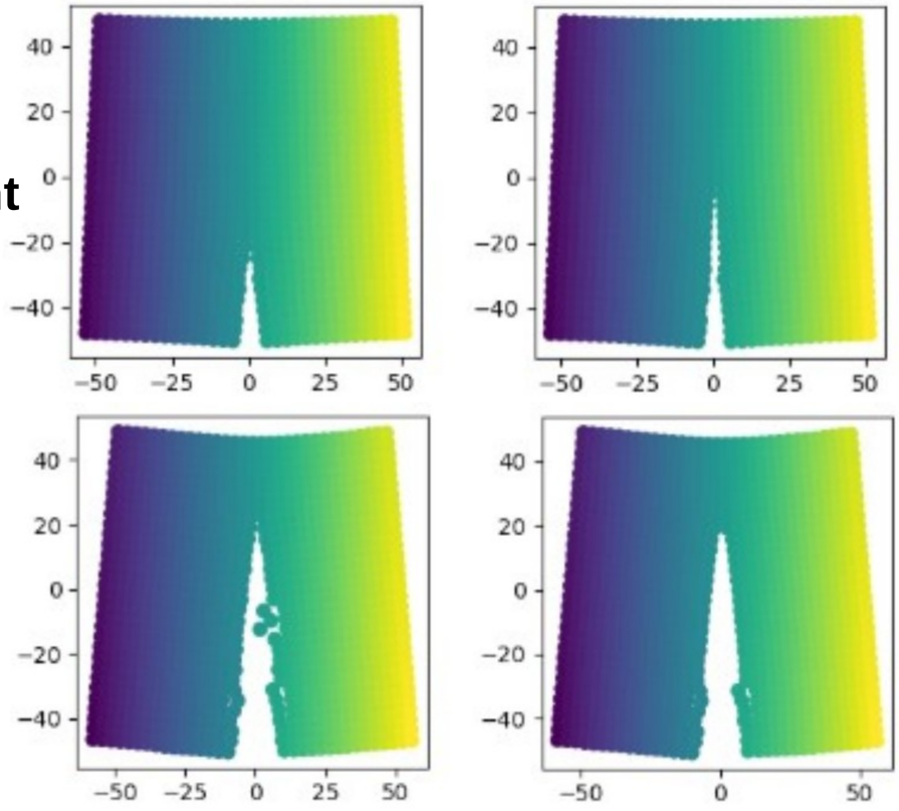
displacement at 20 steps

displacement at 40 steps



Prediction at a different resolution

Ground-truth (Δx=2.5) **Prediction (Δx=2.5)**



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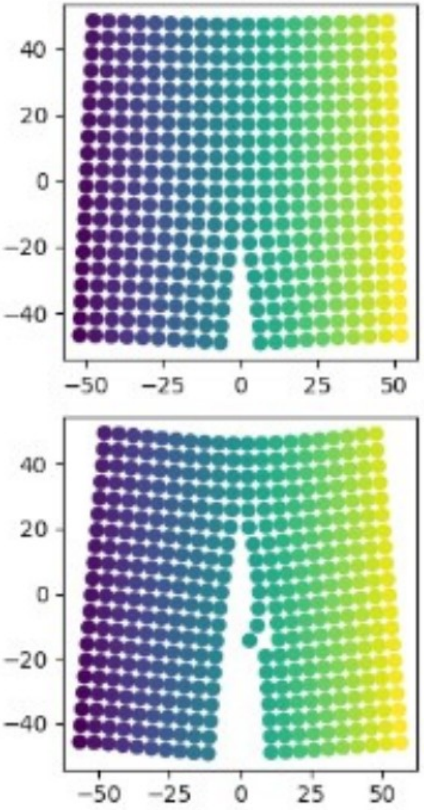
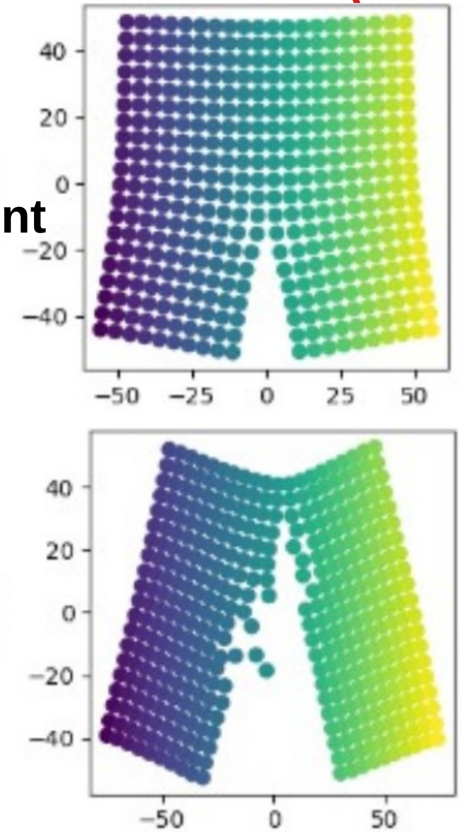
displacement at 20 steps

displacement at 40 steps

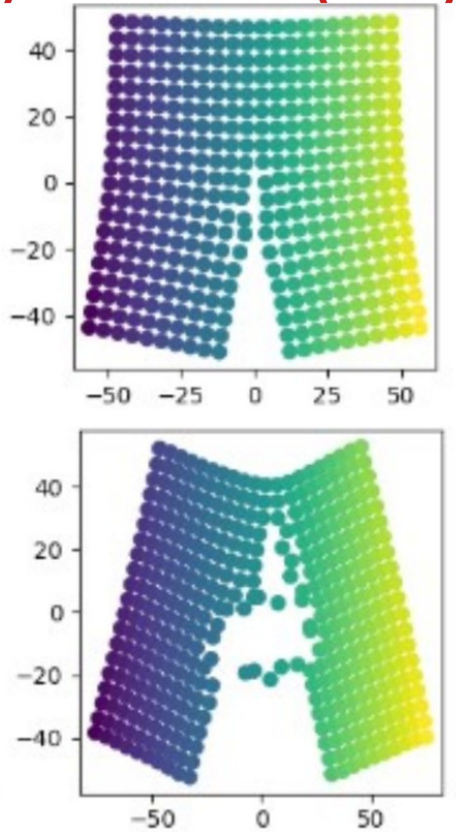


Prediction at a different loading

Ground-truth (Δx=5)



Prediction (Δx=5)



Part II
Learning Nonlocal Constitutive Laws with Neural Operator

[1] S. Jafarzadeh, S. Silling, N. Liu, Z. Zhang, Y. Yu*, "Neural Peridynamic Operators: A Data-Driven Nonlocal Constitutive Model for Complex Material Responses". In preprint.

[2] N. Liu, Y. Yu*, H. You, N. Tatikola. "INO: Invariant Neural Operator for Learning Complex Physical Systems with Momentum Conservation", AISTATS, 2023

[3] L. Zhang, H. You, T. Gao, M. Yu, C-H. Lee, **Y. Yu***, "MetaNO: How to Transfer Your Knowledge on Learning Hidden Physics", CMAME, 2023.

[4] H. You, Q. Zhang, C. Ross, C-H. Lee, M-C. Hsu, **Y. Yu***, "A Physics-Guided Neural Operator Learning Approach to Model Biological Tissues from Digital Image Correlation Measurements". Journal of Biomechanical Engineering, 2022.

Generic Nonlocal Constitutive Law

- **Goal:** identify a nonlocal integrant in $\mathcal{G}[\mathbf{u}](\mathbf{x},t) := \int_{B_\delta(\mathbf{x})} \mathbf{b}(\mathbf{y},\mathbf{x},\mathbf{u},t)\, d\mathbf{y}$

s.t.,
$$\begin{cases} \rho\ddot{\mathbf{u}} = \mathcal{G}_{[k,\underline{\mathbf{T}},d]}\mathbf{u} + \mathbf{f} & \text{in } \Omega \\ \mathbf{u} = \mathbf{u}_{bc} & \text{on the nonlocal boundary } \Omega_\delta \end{cases}$$

1) **Collect measurements** of function pairs: $\mathcal{D} = \{\mathbf{u}_j(\mathbf{x},t), \mathbf{f}_j(\mathbf{x},t)\}_{j=1}^N$

Training set: measurements or high fidelity simulations

2) **Approximate the integrant** with a parameterization:

Generic model[2] $\mathbf{b}(\mathbf{y},\mathbf{x},\mathbf{u},t) := \underline{\mathbf{T}}(\mathbf{x},\mathbf{y},\mathbf{u})d(\mathbf{x},\mathbf{y},\mathbf{u},t)$

Idea: parameterize *G* with a Nonlocal Neural Operator

Outcomes:
1. material-specific kernel function k, force state $\underline{\mathrm{T}}$, and damage field d.
2. the surrogate model
$$\mathcal{G}_{[k,\underline{\mathbf{T}}]}\mathbf{u} = \mathbf{f}$$
for downstream tasks.

3) **Minimize the residual**

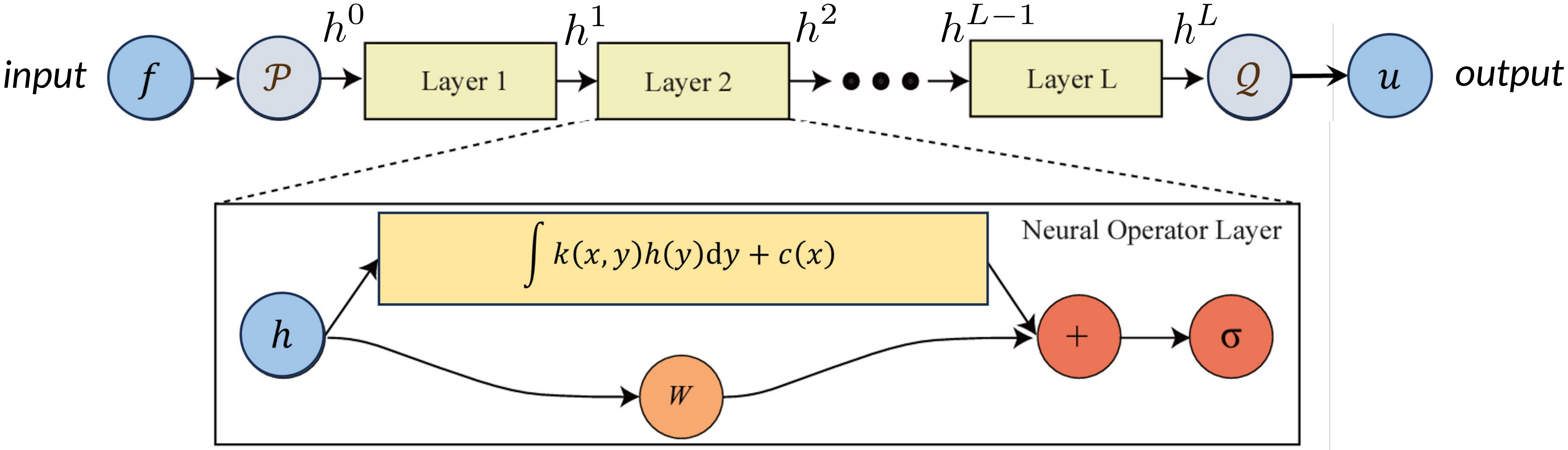
$$\mathcal{E}_\lambda(k,\underline{\mathbf{T}},d) = \frac{1}{N}\sum_{j=1}^{N} \|\mathcal{G}_{[k,\underline{\mathbf{T}},d]}[\mathbf{u}_j] + \mathbf{f}_j - \rho\ddot{\mathbf{u}}_j\|_{L^2}^2 + \lambda\mathcal{R}(k,\underline{\mathbf{T}},d)$$

[1]Liu, Ning, Siavash Jafarzadeh, and Yue Yu. "Domain Agnostic Fourier Neural Operators." NeurIPS, 2023

Nonlocal Neural Operators

Idea: design neural networks to model function-to-function mapping

- Features: The learnt model is **generalizable to future prediction tasks, with different loadings and/or different resolutions**.



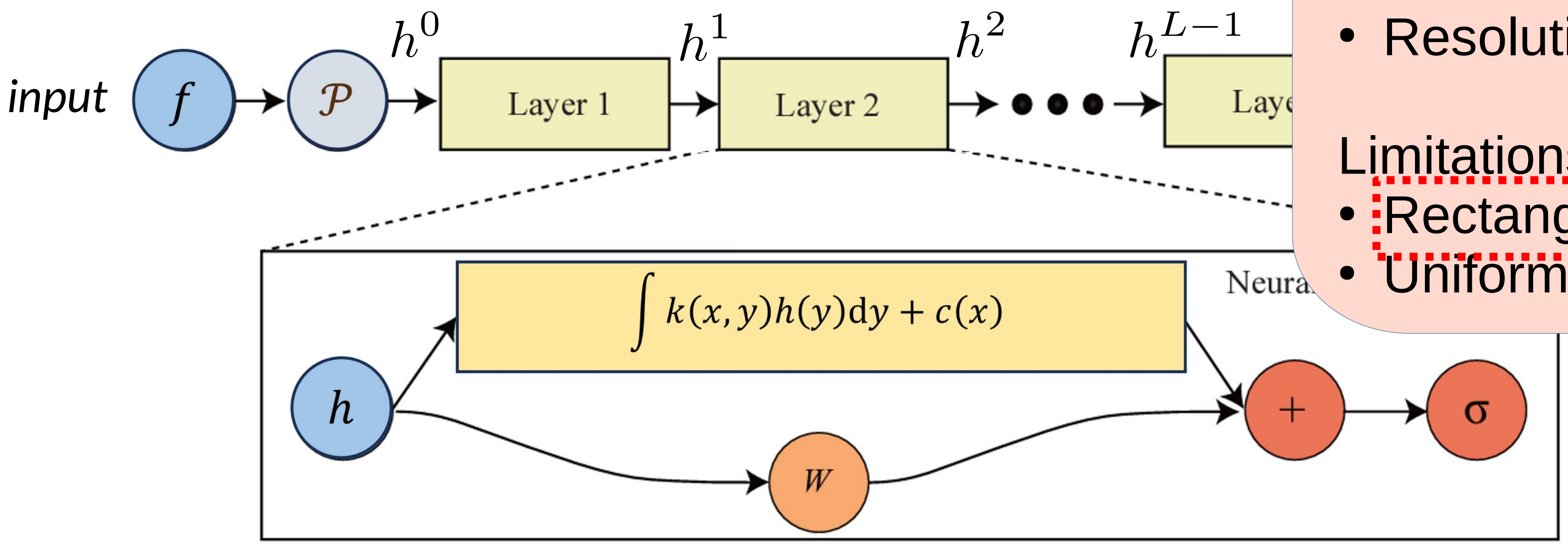
$$\mathbf{h}^{l+1}(\mathbf{x}) = \mathcal{L}^l[\mathbf{h}^l](\mathbf{x}) := \sigma\left(W^l\mathbf{h}^l(\mathbf{x}) + \mathbf{c}^l + \int_\Omega \kappa(\mathbf{x},\mathbf{y};\mathbf{v}^l)\mathbf{h}^l(\mathbf{y})d\mathbf{y}\right)$$

[1]Li, Zongyi, et al. "Fourier Neural Operator for Parametric Partial Differential Equations." International Conference on Learning Representations. 2020.

Fourier Neural Operators

Idea: design neural networks to model function-

- Features: The learnt model is **generalizable to future prediction and/or different resolutions**.



FFT to evaluate integral

Key advantages:
- Efficiency
- Resolution-independence

Limitations:
- Rectangular domain
- Uniform grids

$$\mathbf{h}^{l+1}(\mathbf{x}) = \mathcal{L}^l_{FNO}[\mathbf{h}^l](\mathbf{x}) := \sigma\left(W^l \mathbf{h}^l(\mathbf{x}) + \mathbf{c}^l + \mathcal{F}^{-1}[\mathcal{F}[\kappa(\cdot;\mathbf{v}^l)] \cdot \mathcal{F}[\mathbf{h}^l(\cdot)]](\mathbf{x}) \right)$$

[1]Li, Zongyi, et al. "Fourier Neural Operator for Parametric Partial Differential Equations." International Conference on Learning Representations. 2020.

Generic Nonlocal Constitutive Law

- **Goal:** identify a nonlocal integrant in $\mathcal{G}[\mathbf{u}](\mathbf{x},t) := \int_{B_\delta(\mathbf{x})} \mathbf{b}(\mathbf{y},\mathbf{x},\mathbf{u},t)\, d\mathbf{y}$

s.t., $\begin{cases} \rho\ddot{\mathbf{u}} = \mathcal{G}_{[k,\underline{\mathbf{T}},d]}\mathbf{u} + \mathbf{f} & \text{in } \Omega \\ \mathbf{u} = \mathbf{u}_{bc} & \text{on the nonlocal boundary } \Omega_{\mathcal{I}} \end{cases}$

1) **Collect measurements** of function pairs: $\mathcal{D} = \{\mathbf{u}_j(\mathbf{x},t), \mathbf{f}_j(\mathbf{x},t)\}_{j=1}^N$

2) **Approximate the integrant** with a parameterization:

Generic model² $\mathbf{b}(\mathbf{y},\mathbf{x},\mathbf{u},t) := \underline{\mathbf{T}}(\mathbf{x},\mathbf{y},\mathbf{u})d(\mathbf{x},\mathbf{y},\mathbf{u},t)$

Idea: parameterize G with an FNO:

$$\mathcal{G}[\mathbf{u}] := \mathcal{Q} \circ \mathcal{L}^L \cdots \mathcal{L}^0 \circ \mathcal{P}[\mathbf{u}]$$

3) **Minimize the residual**

$$\mathcal{E}_\lambda(k,\underline{\mathbf{T}},d) = \frac{1}{N}\sum_{j=1}^{N} \|\mathcal{G}_{[k,\underline{\mathbf{T}},d]}[\mathbf{u}_j] + \mathbf{f}_j - \rho\ddot{\mathbf{u}}_j\|_{L^2}^2 + \lambda\mathcal{R}(k,\underline{\mathbf{T}},d)$$

Advantages:
1. FNO is a universal approximator
2. Efficiency

Challenge:
1. Need to handle complicated and evolving domains

1. material-specific kernel function k, force state T, and damage field d.
2. the surrogate model $\mathcal{G}_{[k,\underline{\mathbf{T}}]}\mathbf{u} = \mathbf{f}$ for downstream tasks.

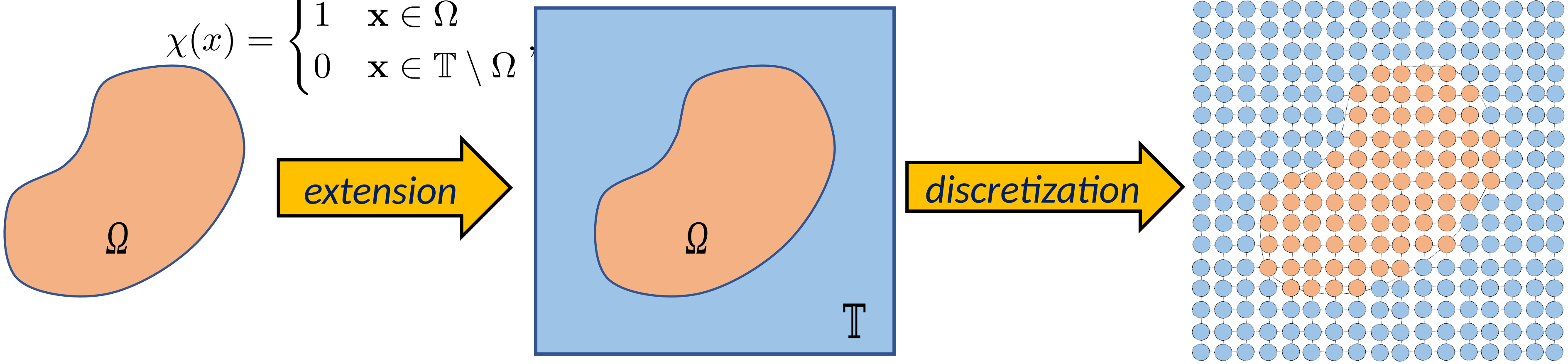
[1] Liu, Ning, Siavash Jafarzadeh, and Yue Yu. "Domain Agnostic Fourier Neural Operators." NeurIPS, 2023

Domain Agnostic FNOs

Goal: design FNO for geometry and topology changes

- **Key idea 1**: **Encode the geometry information into the integral layer**, using the characteristic function χ(**x**), while **retaining the convolutional architecture**.

$$\chi(x) = \begin{cases} 1 & \mathbf{x} \in \Omega \\ 0 & \mathbf{x} \in \mathbb{T} \setminus \Omega \end{cases},$$



$$\mathbf{h}^{l+1}(\mathbf{x}) = \mathcal{L}^l_{DAFNO}[\mathbf{h}^l](\mathbf{x}) := \sigma\left(W^l \mathbf{h}^l(\mathbf{x})\chi(\mathbf{x}) + \mathbf{c}^l \chi(\mathbf{x}) + \int_\Omega \chi(\mathbf{x})\chi(\mathbf{y})\kappa(\mathbf{x}-\mathbf{y};\mathbf{v}^l)(\mathbf{h}^l(\mathbf{y}) - \mathbf{h}^l(\mathbf{x}))d\mathbf{y} \right)$$

$$= \sigma\left(\chi(\mathbf{x}) \left(W^l \mathbf{h}^l(\mathbf{x}) + \mathbf{c}^l + \mathcal{F}^{-1}[\mathcal{F}[\kappa(\cdot;\mathbf{v}^l)] \cdot \mathcal{F}[\chi(\cdot)\mathbf{h}^l(\cdot)]](\mathbf{x}) - \mathbf{h}^l(\mathbf{x})\mathcal{F}^{-1}[\mathcal{F}[\kappa(\cdot;\mathbf{v}^l)] \cdot \mathcal{F}[\chi(\cdot)]](\mathbf{x}) \right)\right).$$

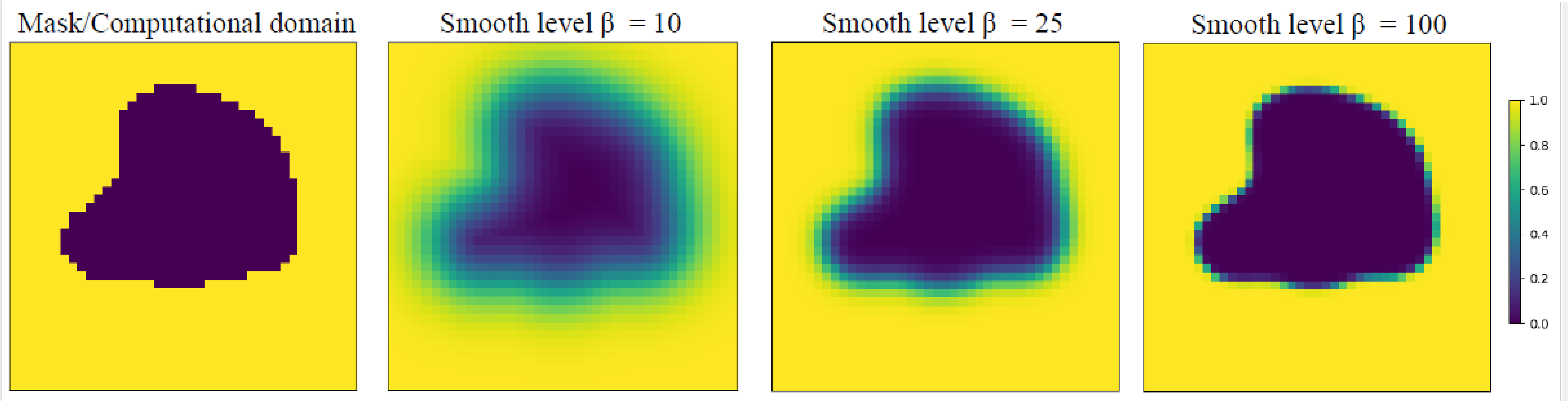
[1]Liu, Ning, Siavash Jafarzadeh, and Yue Yu. "Domain Agnostic Fourier Neural Operators." NeurIPS, 2023

Domain Agnostic FNOs

Goal: design FNO for geometry and topology changes

- **Key idea 2**: Employ a **smoothed characteristic function** χ(**x**), to avoid the Gibbs phenomenon:

$$\tilde{\chi}(\mathbf{x}) := \tanh(\beta \text{dist}(\mathbf{x}, \partial\Omega))(\chi(\mathbf{x}) - 0.5) + 0.5$$



$$\mathbf{h}^{l+1}(\mathbf{x}) = \sigma\left(\tilde{\chi}(\mathbf{x})\left(W^l\mathbf{h}^l(\mathbf{x}) + \mathbf{c}^l + \mathcal{F}^{-1}[\mathcal{F}[\kappa(\cdot;\mathbf{v}^l)]\cdot\mathcal{F}[\tilde{\chi}(\cdot)\mathbf{h}^l(\cdot)]](\mathbf{x}) - \mathbf{h}^l(\mathbf{x})\mathcal{F}^{-1}[\mathcal{F}[\kappa(\cdot;\mathbf{v}^l)]\cdot\mathcal{F}[\tilde{\chi}(\cdot)]](\mathbf{x})\right)\right).$$

[1] Liu, Ning, Siavash Jafarzadeh, and Yue Yu. "Domain Agnostic Fourier Neural Operators." NeurIPS, 2023 (This paper).

Generic Nonlocal Constitutive Law

- **Goal:** identify a nonlocal integrant in $\mathcal{G}[\mathbf{u}](\mathbf{x},t) := \int_{B_\delta(\mathbf{x})} \mathbf{b}(\mathbf{y},\mathbf{x},\mathbf{u},t)\, d\mathbf{y}$

s.t.,
$$\begin{cases} \rho\ddot{\mathbf{u}} = \mathcal{G}_{[k,\underline{\mathbf{T}},d]}\mathbf{u} + \mathbf{f} & \text{in } \Omega \\ \mathbf{u} = \mathbf{u}_{bc} & \text{on the nonlocal boundary } \Omega_\delta \end{cases}$$

1) **Collect measurements** of function pairs

without damage: $\mathcal{D} = \{\mathbf{u}_j(\mathbf{x},t), \mathbf{f}_j(\mathbf{x},t)\}_{j=1}^N$, and with damage: $\tilde{\mathcal{D}} = \{\tilde{\mathbf{u}}_j(\mathbf{x},t), \tilde{\mathbf{f}}_j(\mathbf{x},t)\}_{j=1}^{\tilde{N}}$.

Training set: measurements or high fidelity simulations

2) **Approximate the integrant** with a parameterization:

Generic model[2] $\mathcal{G}[\mathbf{u}] := \mathcal{Q} \circ \mathcal{L}^L_{\mathrm{D}AFNO}[\chi(d)] \cdots \mathcal{L}^0_{\mathrm{D}AFNO}[\chi(d)] \circ \mathcal{P}[\mathbf{u}]$

3) **Step 1: Pre-train the neural operator on D.**

Step 2: Fine-tune the neural operator on $\tilde{\mathrm{D}}$.

$$\mathcal{E}_\lambda(k,\underline{\mathbf{T}},d) = \frac{1}{N}\sum_{j=1}^{N} \|\mathcal{G}_{[k,\underline{\mathbf{T}},d]}[\mathbf{u}_j] + \mathbf{f}_j - \rho\ddot{\mathbf{u}}_j\|^2_{L^2} + \lambda\mathcal{R}(k,\underline{\mathbf{T}},d)$$

Outcomes:
1. material-specific kernel function k, force state $\underline{\mathrm{T}}$, and damage field d.
2. the surrogate model
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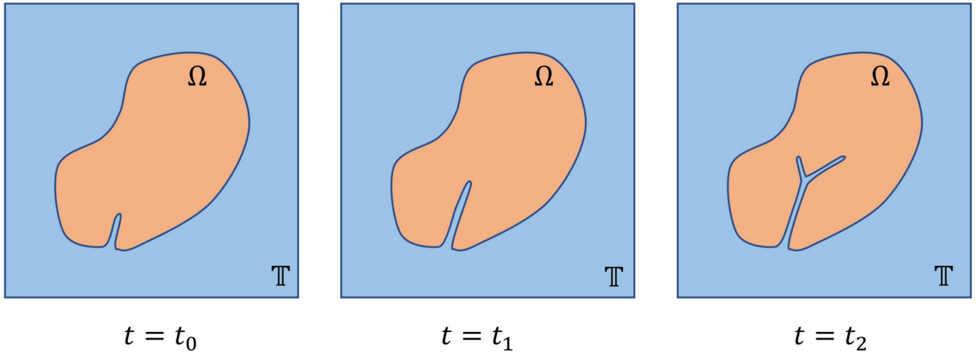
for downstream tasks.

[1]Liu, Ning, Siavash Jafarzadeh, and Yue Yu. "Domain Agnostic Fourier Neural Operators." NeurIPS, 2023

DAFNO: Crack Propagation Prediction



- **Goal:** learn the constitutive model and use it to predict crack propagation.

- **Training data setting:**
  1) Dataset without damage: 2048 sinusoidal data pairs

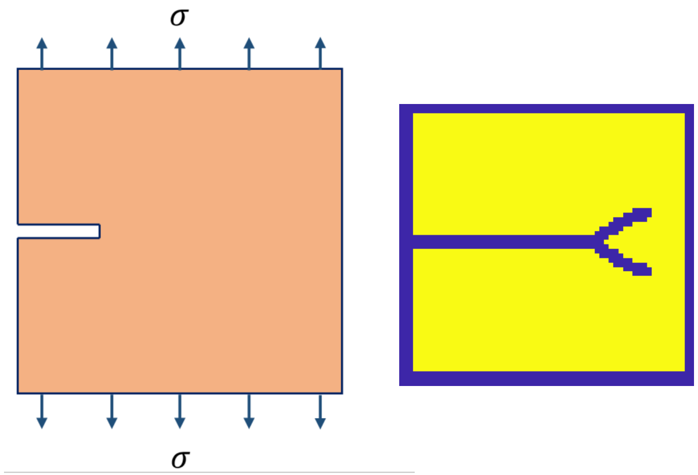
$$
1024 \left\{ \begin{aligned} u_1 &= c \sin\left(m \frac{2\pi x_1}{L}\right) \sin\left(n \frac{2\pi x_2}{L}\right), \\ u_2 &= 0 \end{aligned} \right.
$$

$$
+
$$

$$
1024 \left\{ \begin{aligned} u_1 &= 0 \\ u_2 &= c \sin\left(m \frac{2\pi x_1}{L}\right) \sin\left(n \frac{2\pi x_2}{L}\right) \end{aligned} \right.
$$

for $m, n = 1, 2, \ldots, 32$

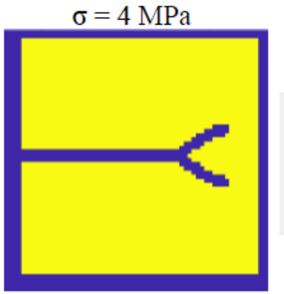
  2) Dataset with damage: A thin plate with a pre-crack subjected to a fixed traction of 4 Mpa (450 snapshots in total)



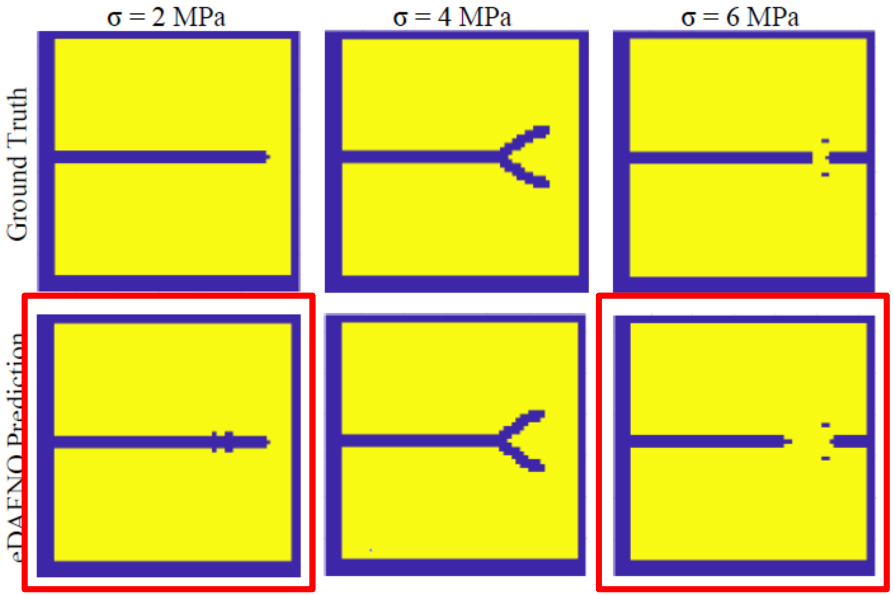
DAFNO: Crack Propagation Prediction

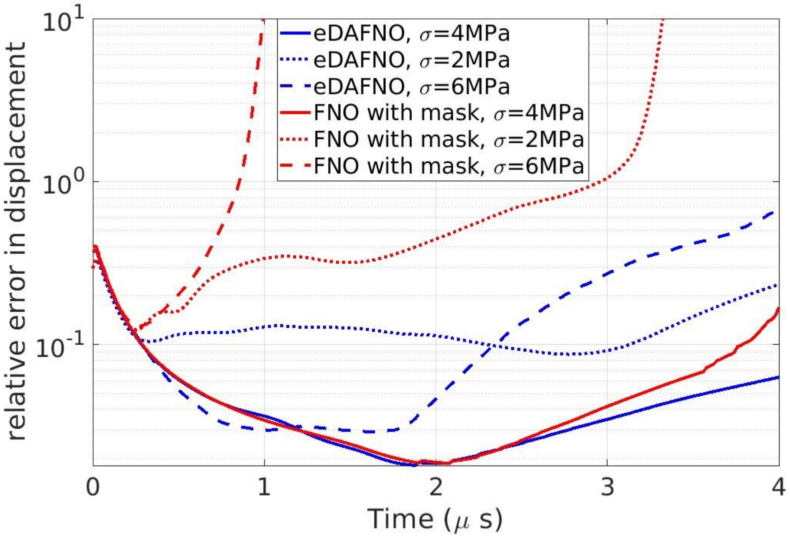
- **Training data setting:**
  A thin plate with a pre-crack subjected to a different fixed traction (2MPa and 6MPa)
  With loading magnitudes and crack patterns not seen from training.

Training data



Test data (unseen topology!)

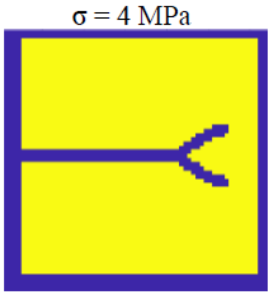




DAFNO: Crack Propagation Prediction

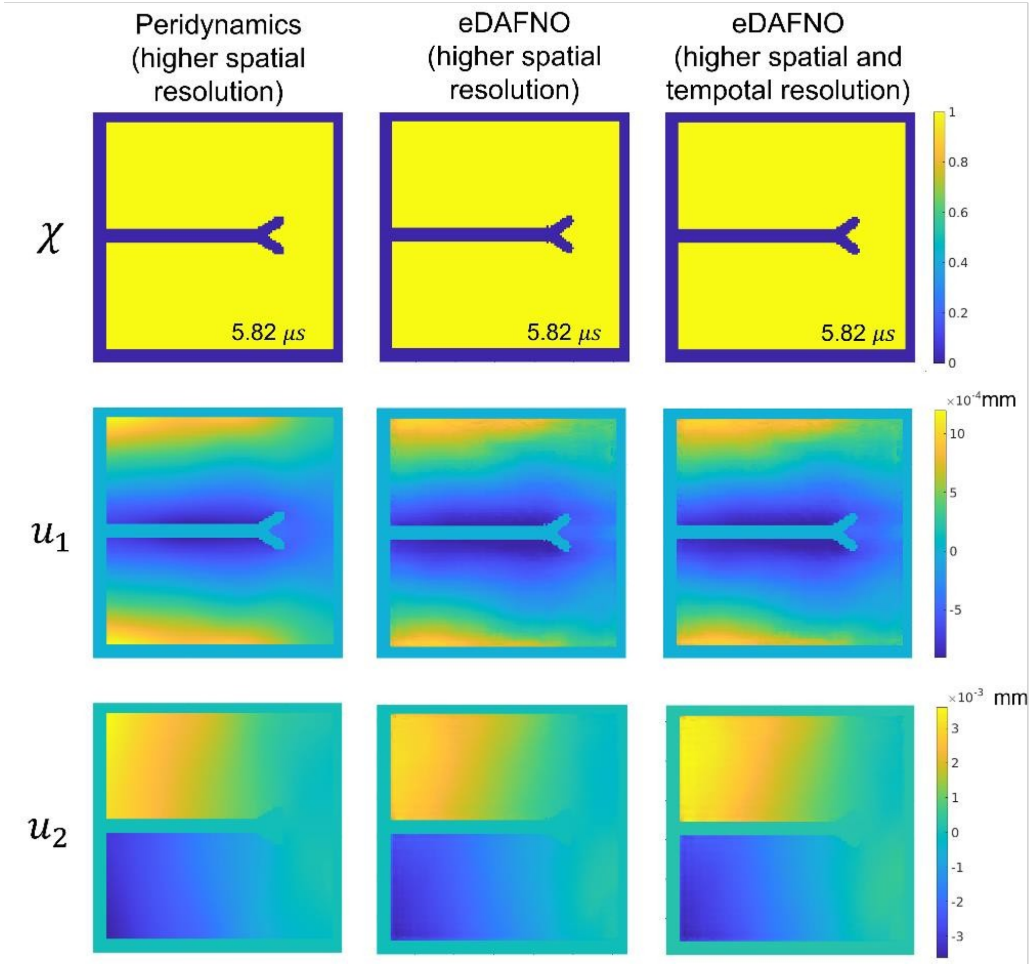
- **Cross-resolution test:**
  Use the trained model to perform zero-shot prediction on a different resolution.

Training data



Training dataset
Resolution: 64 × 64
Δt = 0.02 μs

Predictions on
Resolution: 128 × 128
Δt = 0.01 μs



Takeaways

- We proposed a **nonlocal constitutive law** learning framework, which learns **continuous integrants** for material learning tasks.
- For **linear & homogenized model learning tasks**, the **nonlocal operator regression (NOR) model** is proposed, which learns optimal kernel functions and damage criteria directly from data.
- For **nonlinear & generic material modeling tasks**, the **domain agnostic FNO (DAFNO) model** is proposed, which is geometry-generalizable and hence is capable to evolve the computational domain with fracture.
- The learnt nonlocal constitutive laws are **generalizable to different geometries, resolutions and loading scenarios**.
- Future work: impose physics knowledge in DAFNO.

Thank you!

- **Collaborators:**

  Huaiqian You, Lu Zhang (Ph.D. student), **Siavash Jafarzadeh** (postdoc), *Lehigh University*

  Ning Liu*, GEM;* Stewart Silling, *Sandia;* Marta D’Elia, *Pasteur Labs;* Xu Xiao, John Foster, *UT Austin.*

- **Funding support:**

  NSF CAREER award DMS1753031

  AFOSR YIP grant FA9550-22-1-0197

- **Computational Resources:** Lehigh HPC systems

- **References:**

[1] H. You, Y. Yu*, S. Silling, M. D’Elia, “A data-driven peridynamic continuum model for upscaling molecular dynamics”. CMAME, 2022.
[2] Liu, N, S. Jafarzadeh, and Y. Yu*. "Domain Agnostic Fourier Neural Operators." NeurIPS, 2023
[3] You, H., Xu, X., Yu, Y.*, Silling, S., D'Elia, M., Foster, J. Towards a unified nonlocal, peridynamics framework for the coarse-graining of molecular dynamics data with fractures. Applied Mathematics and Mechanics, 2023.
[4] S. Jafarzadeh, S. Silling, N. Liu, Z. Zhang, Y. Yu*, “Peridynamic Neural Operators: A Data-Driven Nonlocal Constitutive Model for Complex Material Responses”. Under review. 2024.