AI-based identification of coupling regions for local and non-local one-dimensional coupling approaches

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Motivation

Challenges

- Peridynamic simulations are computational expensive
- Applying local boundary conditions in non-local models is not trivial

Solution

- Coupling of non-local and local models
  - Apply boundary conditions in the local region
  - Apply peridynamics in the **region** where we have crack and fractures

Can we use machine learning to identify the peridynamic region?

Overview

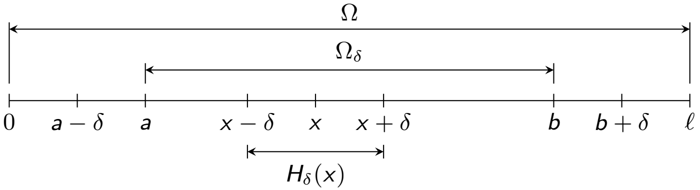
Model problem

Model Problem

Classical linear elasticity model in 1D (with cross-sectional area $A = 1$):

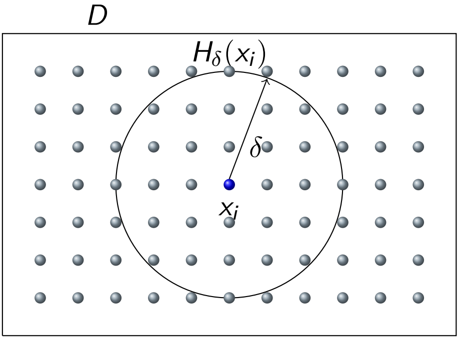
$$\begin{aligned} -E\underline{u}''(x) &= f_b(x), \quad \forall x \in \Omega = (0, \ell), \\ \underline{u}(x) &= 0, \quad \text{at } x = 0 \\ E\underline{u}'(x) &= g, \quad \text{at } x = \ell \end{aligned}$$

Coupling with peridynamic model:
Nonlocal model in $\Omega_\delta = (a, b) \subset \Omega$ where $\delta =$ horizon.



Peridynamics

Peridynamics



- A non-local alternative formulation of classical continuum mechanics
- No differentials of displacement fields are used, which makes it an attractive framework for modeling and simulating fracture mechanics applications.

References

Silling, Stewart A. "Reformulation of elasticity theory for discontinuities and long-range forces." Journal of the Mechanics and Physics of Solids 48.1 (2000): 175-209.

Linearized microelastic bond-based model

$$-\int_{H_\delta(x)} \kappa \frac{\xi \otimes \xi}{\|\xi\|^3}(u(y)-u(x))dy = f_b(x)$$

In 1D:

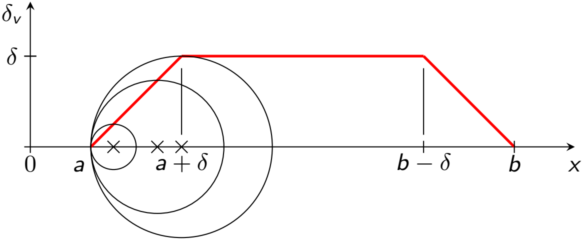
$$\boxed{-\int_{x-\delta}^{x+\delta} \kappa \frac{u(y)-u(x)}{|y-x|}dy = f_b(x)}$$

By taking the limit $\delta \to 0$, one then recovers the local model pointwise whenever κ is chosen as:

$$\boxed{E = \frac{\kappa\delta^2}{2}} \quad \text{i.e.} \quad \boxed{\kappa = \frac{2E}{\delta^2}}$$

Variable Horizon Coupling Approach

VHCM formulation



Variable horizon function:

$$\delta_v(x) = \begin{cases} x - a, & a < x \le a + \delta \\ \delta, & a + \delta < x \le b - \delta \\ b - x, & b - \delta < x < b \end{cases}$$

$$\boxed{\bar{\kappa}(x)\delta_v^2(x) = \kappa\delta^2, \quad \forall x \in \Omega_\delta}$$

VHCM formulation

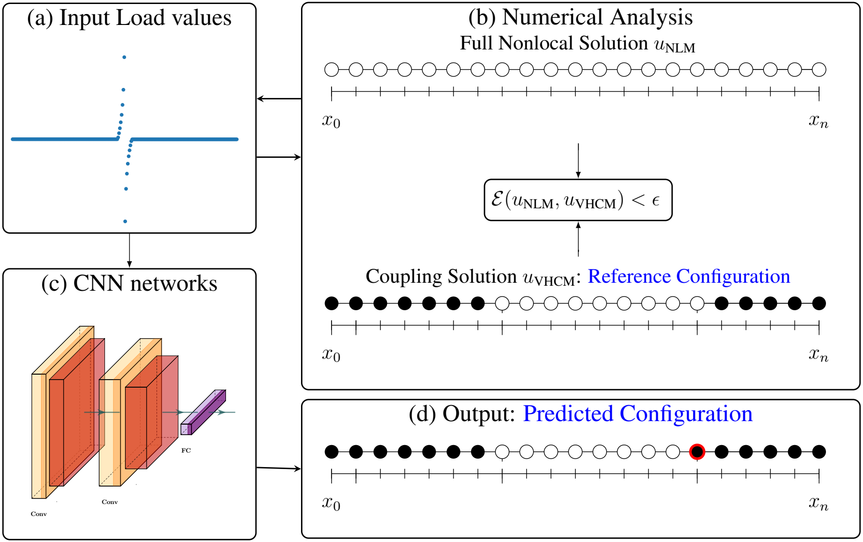
$$
\begin{aligned}
-E\underline{u}''(x) &= f_b(x), \quad \forall x \in \Omega_e \\
-\int_{x-\delta_v(x)}^{x+\delta_v(x)} \bar{\kappa}(x) \frac{u(y)-u(x)}{|y-x|} dy &= f_b(x), \quad \forall x \in \Omega_\delta \\
\underline{u}(x) &= 0, \quad \text{at } x = 0 \\
E\underline{u}'(x) &= g, \quad \text{at } x = \ell \\
u(x) - \underline{u}(x) &= 0, \quad \text{at } x = a, b \\
\sigma^{+}(u)(x) - E\underline{u}'(x) &= 0, \quad \text{at } x = a \\
\sigma^{-}(u)(x) - E\underline{u}'(x) &= 0, \quad \text{at } x = b
\end{aligned}
$$

References

Diehl, Patrick, and Serge Prudhomme. "Coupling approaches for classical linear elasticity and bond-based peridynamic models."

Journal of Peridynamics and Nonlocal Modeling 4.3 (2022): 336-366.

Structure of investigation



Loads used for data generation

The load functions employed in this study include load functions inducing discontinuous solutions with a finite jump at the discontinuity point. The investigation was extended to include the family of loads characterized by solutions of polynomial expressions of degree 3 and lower; which induce full local behavior.

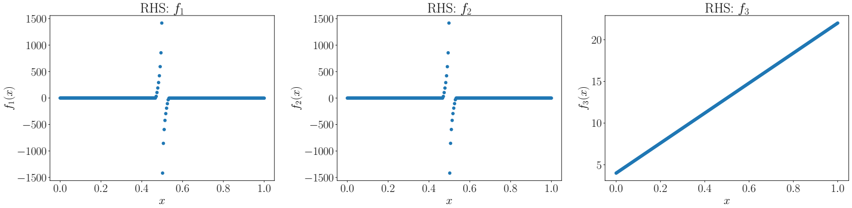
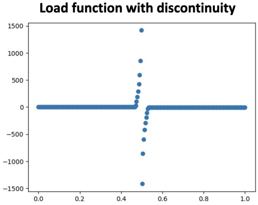


Figure: RHS functions $f_i(x), i = 1..3$.

Load function

$$u(x) = \begin{cases} x & \text{for } x < 0.5 \\ x^2 & \text{for } x > 0.5 \end{cases}$$



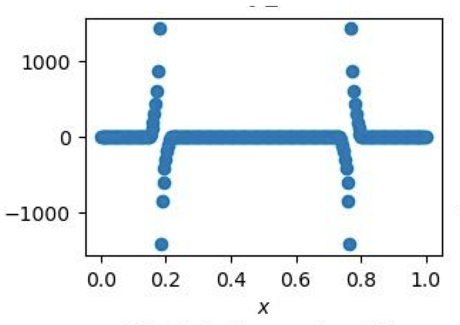
$$f(x) = \begin{cases} 0 & \text{for } x \in [0, 0.5) \\ \frac{1}{2}\delta^2 - \delta + \frac{3}{8} + (2\delta - \frac{3}{2} - \ln\delta)x \\ \quad +(\frac{3}{2} + \ln\delta)x^2 - (x^2 - x)(\ln\frac{1}{2} - x) & \text{for } x \in [0.5 - \delta, 0.5) \\ \frac{1}{2}\delta^2 - \delta + \frac{3}{8} + (2\delta + \frac{3}{2} + \ln\delta)x \\ \quad -(\frac{3}{2} + \ln\delta)x^2 + (x^2 - x)(\ln\frac{1}{2} - x) & \text{for } x \in [0.5, 0.5 + \delta) \\ 1 & \text{for } x \in [0.5 + \delta, 1.0] \end{cases}$$

How to parameterize the NLM region?

The easiest solution: Let the ML model predict the discrete location a and b and all discrete nodes between these points are NLM nodes.

Load function

With multiple discontinuities



How to define the NLM region?

- We can not use *a* and *b* easily since we have multiple intervals depending on the location of the two jumps.
- A more general solution is to predict whether each discrete node is located in local region (LM node) or in the nonlocal region (NLM node).

Numerical Data Simulation

Numerical Data Simulation

- **Parameter Exploration**
  - Central positions of the NLM region vary between 2δ and $l - 2\delta$
  - Adjust coupling region length from h to 0.7
- **Simulation Steps**
  - Execute coupling solution u_{VHCM}
  - Run full nonlocal solution u_{NLM}
  - Estimate error between both solutions: $\mathcal{E}(u_{\text{NLM}}, u_{\text{VHCM}})$
- **Quality Control**
  - Include in dataset solutions with error below tolerance
- **Boundary Conditions**
  - Maintain δ layer at both ends for finite differences
- **Case Studies**

Example of Data Simulation

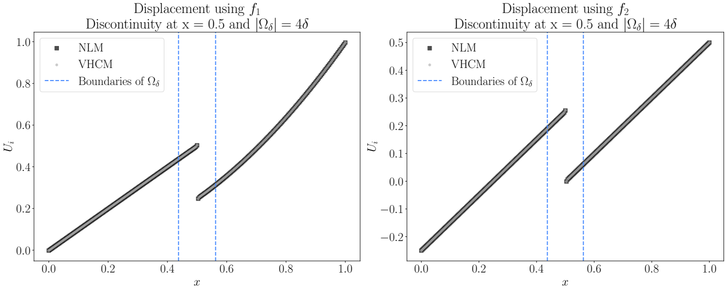


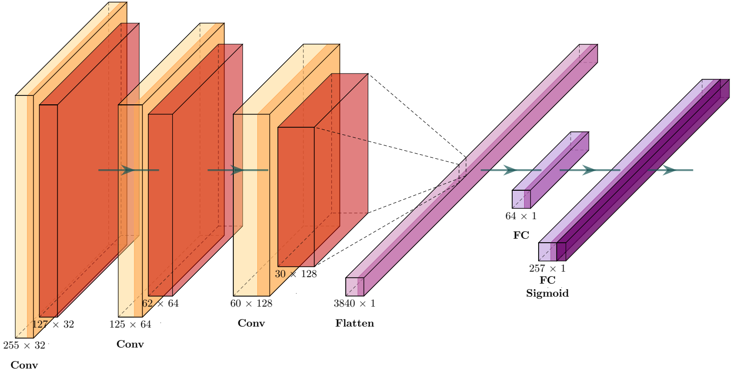
Figure: Peridynamic region configuration with discontinuity at $x = 0.5$. u_{NLM} is represented by ■ and u_{VHCM} is represented by •; (Left) displacement fields u_{NLM} and u_{VHCM} using load f_1; (Right) displacement fields u_{NLM} and u_{VHCM} using load f_2. In both cases, the two curves coincide.

With the following error estimation:

- $\mathcal{E}_{f_1}(u_{\mathrm{NLM}}, u_{\mathrm{VHCM}}) = 4.206 \times 10^{-3}$.
- $\mathcal{E}_{f_2}(u_{\mathrm{NLM}}, u_{\mathrm{VHCM}}) = 4.207 \times 10^{-3}$.

Machine learning model

Machine learning model: CNN



Results

- **Input**: Full Vector Input
- **Output**: Label (NLM or LM) for each discrete node

	Train	Test	Validation	**Total**
Case 1	2313	463	308	3084

- **Prediction Evaluation:** Estimate nonlocal region borders (a, b) from predicted output -> Solution estimation based on full nonlocal and coupling algorithms -> Error calculation between Full nonlocal and Coupling solution
- **Results:**

	Accuracy	**F1-score**	**Load**	$\mathcal{E}(u_{\textbf{NLM}}, u_{\textbf{VHCM}})$
Case 1	0.99	0.99	f_1	2.17×10^{-6}- 1.40×10^{-2}
			f_2	1.17×10^{-6} - 1.33×10^{-4}

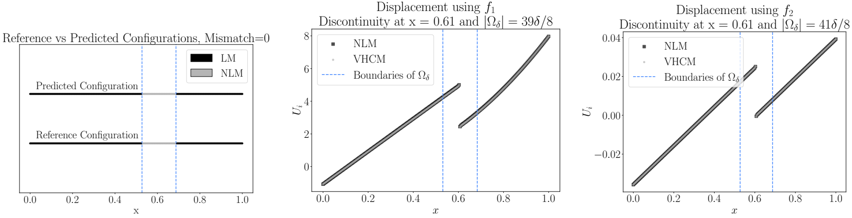
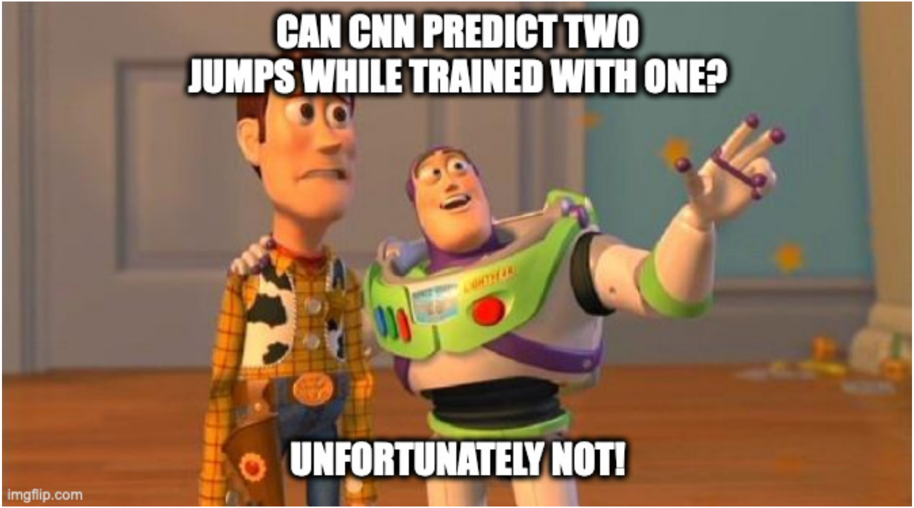


Figure: Error estimation after prediction (a) Comparison between the reference and predicted configurations of local and nonlocal regions. (b) displacement fields u_{NLM} (■) and u_{VHCM} (•) using load f_1. (c) displacement fields u_{NLM} and u_{VHCM} using load f_2.

With the following error estimation:

- $\mathcal{E}_{f_1}(u_{\text{NLM}}, u_{\text{VHCM}}) = 4.036 \times 10^{-4}$.
- $\mathcal{E}_{f_2}(u_{\text{NLM}}, u_{\text{VHCM}}) = 4.035 \times 10^{-4}$.

How good is our CNN for extrapolation?



Windowing

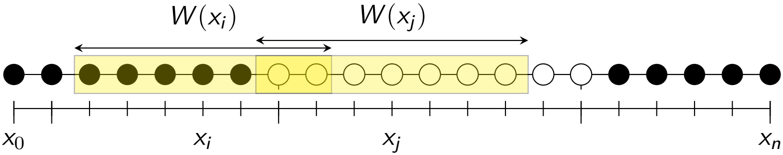


Figure: Schematic representation of data points and their corresponding windows. Two specific data points, x_i and x_j, are highlighted, each associated with its own window, denoted as $W(x_i)$ and $W(x_j)$.

Resulting Dataset:

	Train	Test	Validation	Total
Case 2	109885	22959	15312	148156

- **Input**: Window Input
- **Output**: Label (NLM or LM) for each discrete node
- **Test:** $f_4 = tanh((x - 0.5)/t), t = 0.05$.

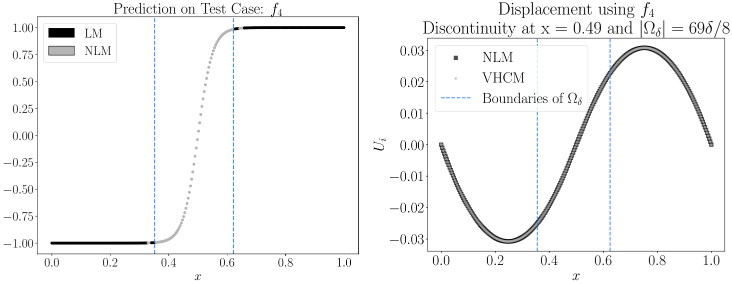


Figure: Nonlocal region detection and error estimation after prediction for general test case

- $\mathcal{E}_{f_4}(u_{NLM}, u_{VHCM}) = 1.73 \times 10^{-4}$.

- **Input**: Window Input
- **Output**: Label (NLM or LM) for each discrete node
- **Test:** $f_4 = tanh((x - 0.5)/t), t = 0.0005$.

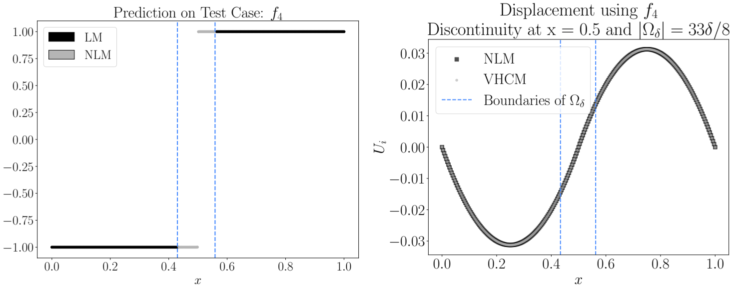


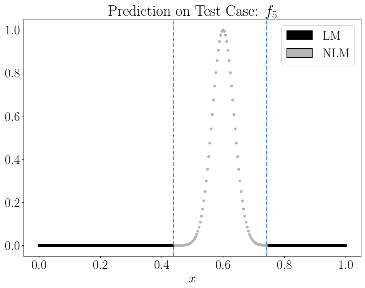
Figure: Nonlocal region detection and error estimation after prediction for general test case

- $\mathcal{E}_{f_4}(u_{NLM}, u_{VHCM}) = 1.75 \times 10^{-4}$.

Results

Case 2: Widowing Data

- **Input**: Window Input
- **Output**: Label (NLM or LM) for each discrete node
- **Test:** $f_5 = e^{-(20x-10-c)^2}, c = 2$



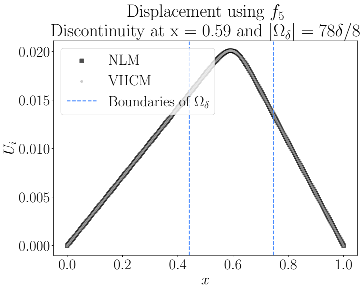


Figure: Nonlocal region detection and error estimation after prediction for general test case

- $\mathcal{E}_{f_5}(u_{NLM}, u_{VHCM}) = 9.93 \times 10^{-5}$.

Summary

Case Study	Case 1	Case 2
Input	Full Vector	Windows
Output	Full Labels Vector	One Node Label
Load Dataset	$f_i(x), \quad i = 1, 2, 3$ and their transformations.	$f_i(x), \quad i = 1, 2, 3$ and their transformations.
ML Model Type	Multiple node Classification	Node wise Classification
Interpretation	Demonstrated the feasibility of the proposed approach for region detection, as a kind of a “proof of concept”.	Highly effective strategy for handling data with varying numbers of discontinuities without the need for retraining the model for each specific scenario.

Outlook and conclusion

Conclusion

- Proof of concept for predicting the coupling region
- Relatively low training data needed

Outlook

- Improve the CNN to generalize our model
- Moving to two dimensions
- Including damage by bond breaking in two dimensions

Paper under Preparation:

AI-based identification of overlapping regions for coupling local and non-local models

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I am happy to take any of your questions.