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Coupling Approaches for Integrating Meshfree Peridynamic Models with Classical Finite Element Analysis

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Outline

BRIEF INTRODUCTION

- Peridynamic model of solid mechanics
- Meshfree discretization scheme of Silling and Askari

VARIABLE LENGTH SCALE IN A PERIDYNAMIC MEDIUM

- Reducing the peridynamic horizon in the vicinity of a local-nonlocal boundary improves model compatibility
- Standard peridynamic models do not support a variable horizon
- The peridynamic partial stress formulation does support a variable horizon and can be utilized for local-nonlocal coupling

OPTIMIZATION-BASED COUPLING

- Model coupling can be cast as an optimization problem
- *Objective function*: Difference between solutions in overlap region
- *Constraints*: Governing equations of the individual models

Collaborators

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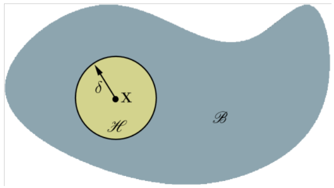
Peridynamic Theory of Solid Mechanics

Peridynamics is a mathematical theory that unifies the mechanics of continuous media, cracks, and discrete particles

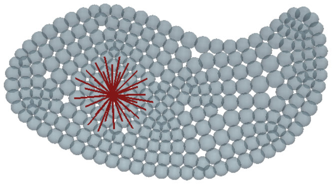
- Peridynamics is a nonlocal extension of continuum mechanics
- Remains valid in presence of discontinuities, including cracks
- Balance of linear momentum is based on an integral equation

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \underbrace{\int_{\mathscr{B}} \left\{ \underline{\mathbf{T}}[\mathbf{x},t]\left\langle \mathbf{x}' - \mathbf{x} \right\rangle - \underline{\mathbf{T}}'[\mathbf{x}',t]\left\langle \mathbf{x} - \mathbf{x}' \right\rangle \right\} \, \mathrm{d}V_{\mathbf{x}'}}_{\text{Divergence of stress replaced with integral of nonlocal forces.}} + \mathbf{b}(\mathbf{x},t)$$



- Peridynamic bonds connect any two material points that interact directly
- Peridynamic forces are determined by force states acting on bonds
- A peridynamic body may be discretized by a finite number of elements

$$\rho(\mathbf{x})\ddot{\mathbf{u}}_h(\mathbf{x},t) = \sum_{i=0}^{N} \left\{ \underline{\mathbf{T}}[\mathbf{x},t]\left\langle \mathbf{x}_i' - \mathbf{x} \right\rangle - \underline{\mathbf{T}}'[\mathbf{x}_i',t]\left\langle \mathbf{x} - \mathbf{x}_i' \right\rangle \right\} \Delta V_{\mathbf{x}_i'} + \mathbf{b}(\mathbf{x},t)$$



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

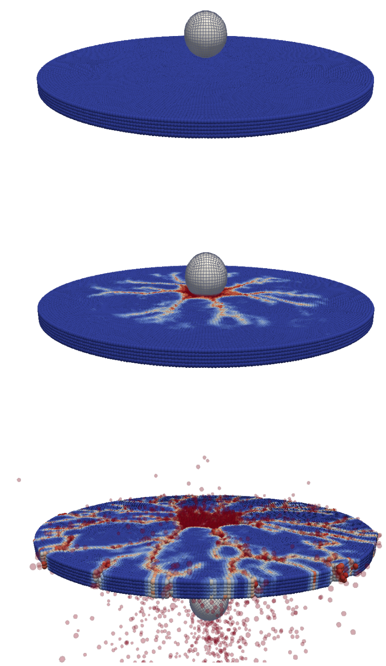
S.A. Silling and E. Askari. A meshfree method based on the peridynamic model of solid mechanics. *Computers and Structures*, 83:1526-1535, 2005.

Silling, S.A. and Lehoucq, R. B. Peridynamic Theory of Solid Mechanics. *Advances in Applied Mechanics* 44:73-168, 2010.

Local-Nonlocal Coupling for Integrated Fracture Modeling

PERIDYNAMICS OFFERS PROMISE FOR MODELING PERVASIVE MATERIAL FAILURE

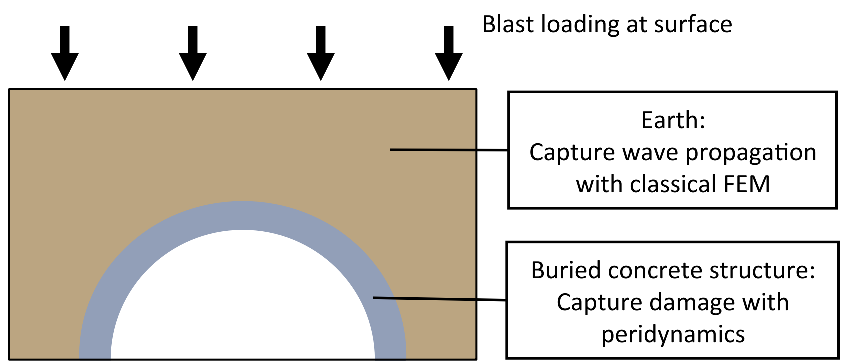
- Potential to enable rigorous simulation of failure and fracture
- Directly applicable to Sandia's national security missions



WE SEEK INTEGRATION WITH CLASSICAL FINITE-ELEMENT APPROACHES

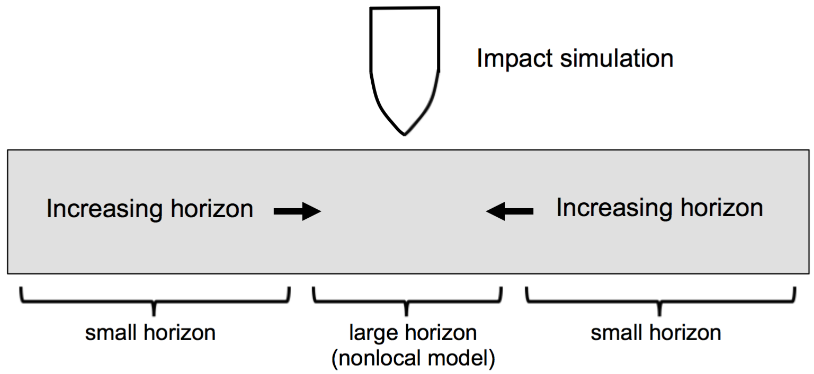
- Integration with existing FEM codes provides a delivery mechanism to DOE and DoD analysts
- "Best of both worlds" through combined classical FEM and peridynamic simulations

Vision
Apply peridynamics in regions susceptible to material failure



Variable Nonlocal Length Scale

Facilitate local-nonlocal coupling in combined peridynamic / classical FEM simulations



STANDARD PERIDYNAMIC MODELS DO NOT SUPPORT A VARIABLE LENGTH SCALE

- Limited support: peridynamic models can support a linearly varying horizon
- *Ghost forces* are proportional to the *second derivative of the horizon*
- Difficulties persist at transition from a constant horizon to a varying horizon

PATH FORWARD

- Seek a formulation that mitigates difficulties associated with a variable horizon
- Target one-dimensional patch tests (expose spurious artifacts, if any)
  - Linear displacement field must be equilibrated
  - Quadratic displacement field must produce constant acceleration

Peridynamic Stress Tensor

ALTERNATIVE EXPRESSION FOR INTERNAL FORCE, TIES TO LOCAL THEORY

Internal force density

$$\mathbf{L}^{\mathrm{pd}}(\mathbf{x}) = \int_{\mathcal{B}} \left\{ \underline{\mathbf{T}}[\mathbf{x}]\langle \mathbf{q} - \mathbf{x} \rangle - \underline{\mathbf{T}}[\mathbf{q}]\langle \mathbf{x} - \mathbf{q} \rangle \right\} dV_{\mathbf{q}}$$

Peridynamic stress tensor [1]

$$\mathbf{L}^{\mathrm{pd}} = \nabla \cdot \boldsymbol{\nu}^{\mathrm{pd}}$$

$$\boldsymbol{\nu}^{\mathrm{pd}}(\mathbf{x}) = \frac{1}{2} \int_{\mathcal{S}} \int_0^{\infty} \int_0^{\infty} (v + w)^2 \mathbf{f}(\mathbf{x} + v\mathbf{m}, \mathbf{x} - w\mathbf{m}) \otimes \mathbf{m} \; dw \; dv \; d\Omega_{\mathbf{m}}$$

where

$$\mathbf{f}(\mathbf{q}, \mathbf{p}) = \underline{\mathbf{T}}[\mathbf{p}]\langle \mathbf{q} - \mathbf{p} \rangle - \underline{\mathbf{T}}[\mathbf{q}]\langle \mathbf{p} - \mathbf{q} \rangle$$

[1] Lehoucq, R.B., and Silling, S.A. Force flux and the peridynamic stress tensor, Journal of the Mechanics and Physics of Solids, 56:1566-1577, 2008.

Peridynamic Partial Stress Formulation

Under the assumption of a **uniform displacement** field

$$\mathbf{y}(\mathbf{x}+\boldsymbol{\xi}) - \mathbf{y}(\mathbf{x}) = \mathbf{F}\boldsymbol{\xi}$$

The peridynamic stress tensor is greatly simplified

$$\begin{aligned}
\boldsymbol{\nu}^{\text{pd}} &= \int_{\mathcal{S}} \int_0^\infty \int_v^\infty z^2 \underline{\hat{\mathbf{T}}}(\underline{\mathbf{F}})\langle z\mathbf{m}\rangle \otimes \mathbf{m}\; dz\; dv\; d\Omega_{\mathbf{m}} \\
&= \int_{\mathcal{S}} \int_0^\infty \int_0^z z^2 \underline{\hat{\mathbf{T}}}(\underline{\mathbf{F}})\langle z\mathbf{m}\rangle \otimes \mathbf{m}\; dv\; dz\; d\Omega_{\mathbf{m}} \\
&= \int_{\mathcal{S}} \int_0^\infty z^3 \underline{\hat{\mathbf{T}}}(\underline{\mathbf{F}})\langle z\mathbf{m}\rangle \otimes \mathbf{m}\; dz\; d\Omega_{\mathbf{m}} \\
&= \int_{\mathcal{S}} \int_0^\infty \underline{\hat{\mathbf{T}}}(\underline{\mathbf{F}})\langle z\mathbf{m}\rangle \otimes (z\mathbf{m})(z^2\; dz\; d\Omega_{\mathbf{m}}) \\
&= \boldsymbol{\nu}^0
\end{aligned}$$

The result is the *peridynamic partial stress*

$$\boldsymbol{\nu}^0 = \int_{\mathcal{H}} \underline{\hat{\mathbf{T}}}(\underline{\mathbf{F}})\langle\boldsymbol{\xi}\rangle \otimes \boldsymbol{\xi}\; dV_{\boldsymbol{\xi}}$$

S.A. Silling, D.J. Littlewood, and P.D. Seleson. Variable Horizon in a Peridynamic Medium. SAND Report 2014-19088. Sandia National Laboratories, Albuquerque, NM and Livermore, CA, 2014.

Peridynamic Partial Stress Formulation

$$\nu_o(\mathbf{x}) := \int_{\mathcal{H}} \underline{\mathbf{T}}[\mathbf{x}]\langle\xi\rangle \otimes \xi \, dV_{\mathbf{x}'}$$

- GOOD: Supports variable horizon
  - Guaranteed to pass the linear patch test (even with a varying horizon)
  - Provides a natural transition between the full peridynamic formulation and a classical stress-strain formulation (hybrid approach)

- BAD: Is exact only for uniform displacement field
  - Partial stress formulation is not a good candidate for modeling material failure
  - Saving grace: we will apply the partial stress only at local-nonlocal coupling interfaces, which are placed in relatively smooth regions

$$\boldsymbol{\nu}^{\mathrm{pd}} - \boldsymbol{\nu}^{\mathrm{ps}} = O(\delta)O(|\nabla\underline{\mathbf{T}}_1|)$$

S.A. Silling, D.J. Littlewood, and P.D. Seleson. Variable Horizon in a Peridynamic Medium. SAND Report 2014-19088. Sandia National Laboratories, Albuquerque, NM and Livermore, CA, 2014.

Application of Partial Stress within Peridynamics Framework

INTERNAL FORCE CALCULATION REQUIRES DIVERGENCE OPERATOR

- Internal force evaluated as divergence of partial stress

$$\mathbf{L}(\mathbf{x}) = \nabla \cdot \nu(\mathbf{x}) = \mathrm{Tr}(\nabla \nu(\mathbf{x}))$$

$$\nabla \nu(\mathbf{x}) = \int_{\mathcal{H}} \underline{\omega}\langle \xi \rangle \{\nu(\mathbf{x}') - \nu(\mathbf{x})\} \otimes \xi \, dV_{\mathbf{x}'} \; \mathbf{K}^{-1}$$

- The partial stress can be applied within the meshless approach of Silling and Askari [1]

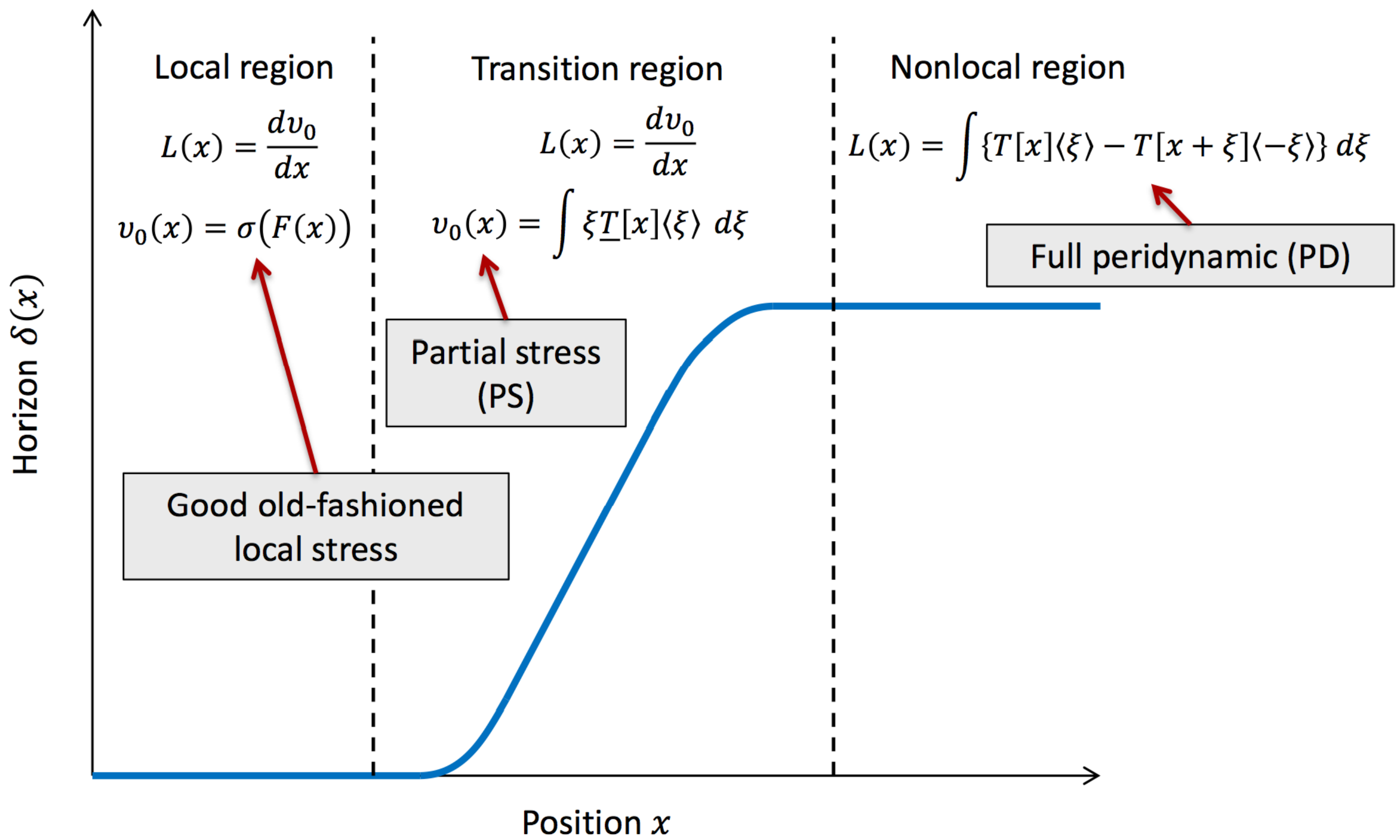
$$\nabla \cdot \nu(\mathbf{x}) = \mathrm{Tr}\left(\left(\sum_{n=1}^{N} \underline{\omega}\langle \xi^n \rangle \{\nu(\mathbf{x}^n) - \nu(\mathbf{x})\} \otimes \xi^n \, \Delta V^n \right) \mathbf{K}^{-1} \right)$$

★ The partial stress can also be applied within a standard finite-element scheme

[1] S.A. Silling and E. Askari. A meshfree method based on the peridynamic model of solid mechanics. *Computers and Structures*, 83:1526-1535, 2005.

Utilize the Partial Stress Formulation in a Transition Region

ALTER THE PERIDYNAMIC HORIZON WITHIN A BODY TO APPLY NONLOCALITY ONLY WHERE NEEDED



[Courtesy Stewart Silling]

Patch Tests for Partial Stress Formulation

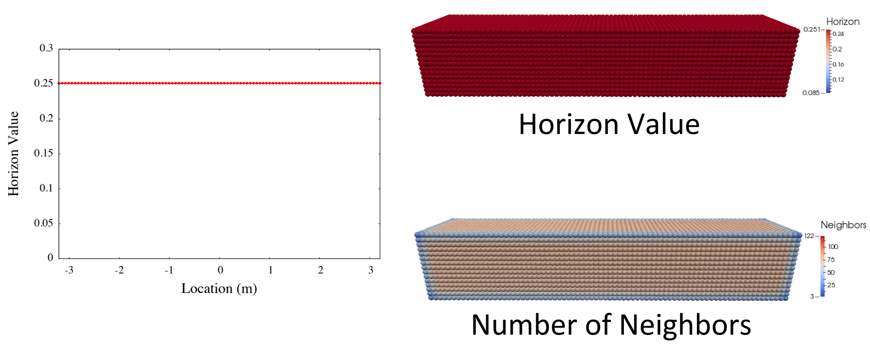
SUBJECT RECTANGULAR BAR TO PRESCRIBED DISPLACEMENT FIELDS

- Examine response under linear and quadratic displacement fields
- Investigate standard formulation with both constant and varying peridynamic horizon
- Investigate partial stress formulation with both constant and varying peridynamic horizon

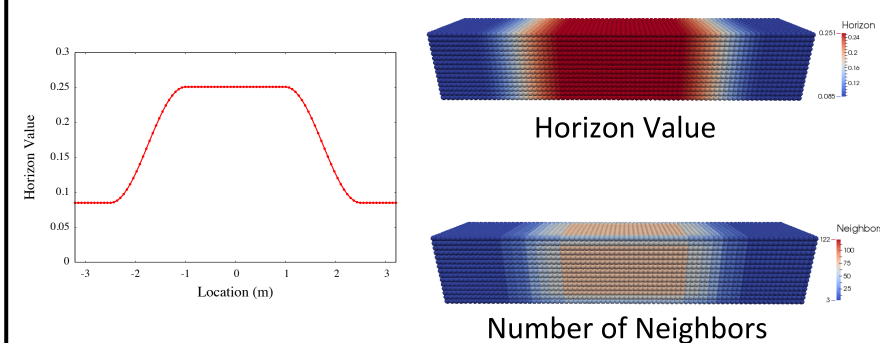
Elastic Correspondence Material Model

Density	7.8 g/cm^3
Young's Modulus	200.0 GPa
Poisson's Ratio	0.0
Stability Coefficient	0.0

Constant Horizon



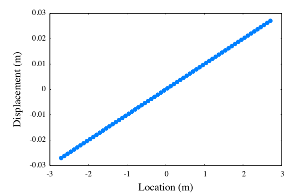
Varying Horizon



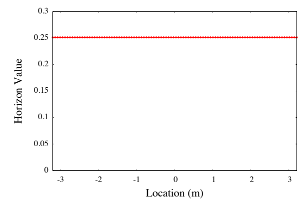
Patch Test: Prescribed Linear Displacement

Test set-up

Prescribe linear displacement field



Constant horizon throughout bar

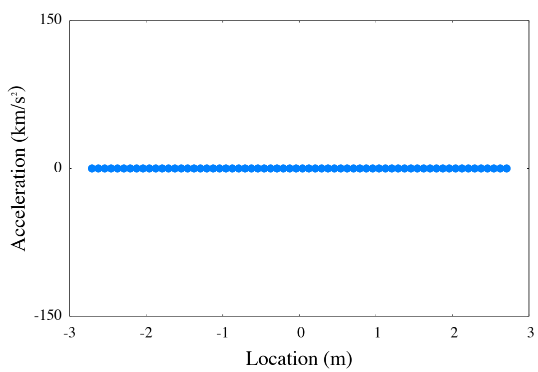


Can the standard model and the partial-stress model recover the expected zero acceleration?

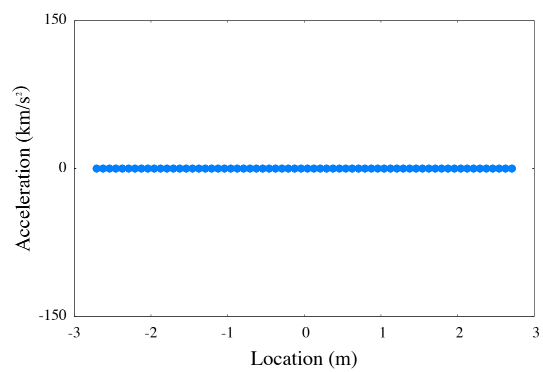
Both models produce the expected result when the horizon is **constant**

Test Results: Acceleration over the length of the bar

Standard material model



Partial-stress formulation

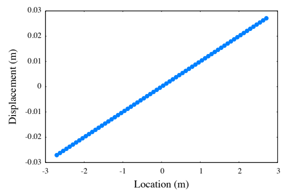


Note: nodes near ends of bar excluded from plots

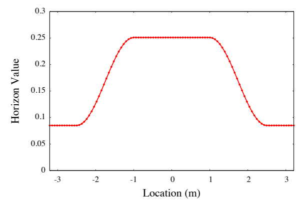
Patch Test: Prescribed Linear Displacement

<u>Test set-up</u>

Prescribe linear displacement field



Variable horizon



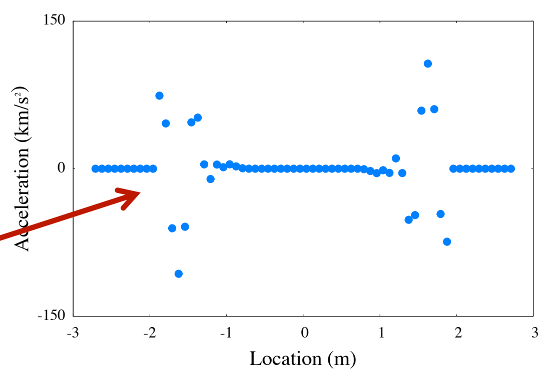
Can the standard model and the partial-stress model recover the expected zero acceleration?

Only the **partial stress** formulation produce the expected result when the horizon is **varying**

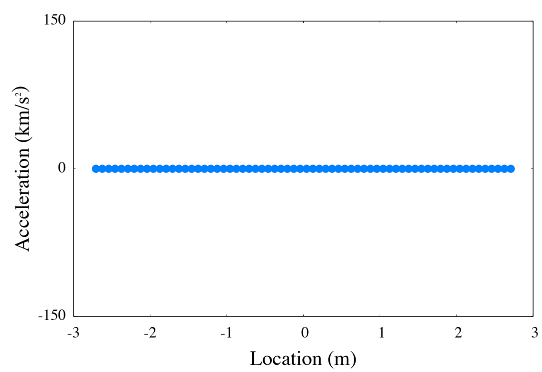
Test Results: Acceleration over the length of the bar

Spurious "ghost forces" present in standard formulation

Standard material model



Partial-stress formulation



Patch Test: Prescribed Quadratic Displacement

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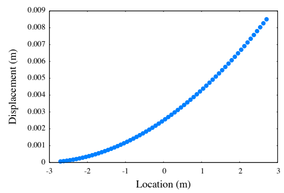
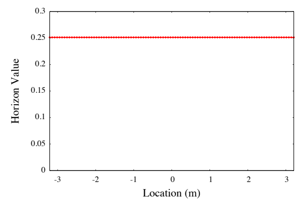
Test set-up

Prescribe quadratic displacement field



Constant horizon throughout bar

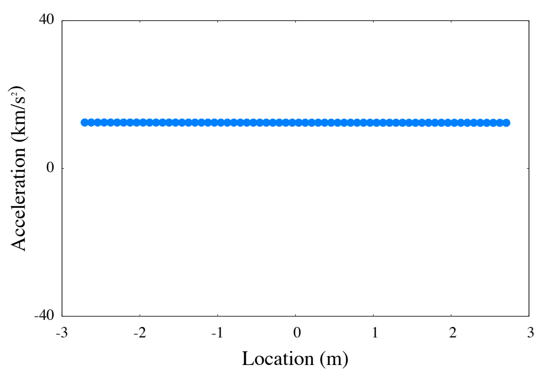


Can the standard model and the partial-stress model recover the expected constant acceleration profile?

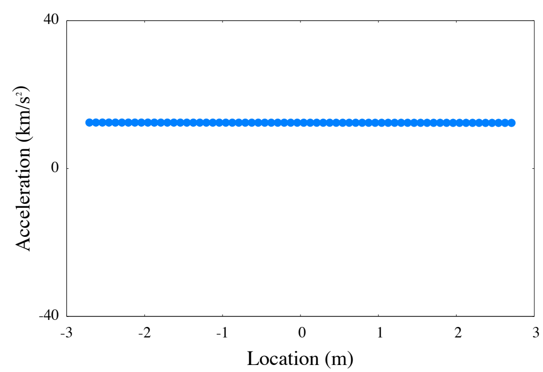
Both models produce the expected result when the horizon is **constant**

Test Results: Acceleration over the length of the bar

Standard material model



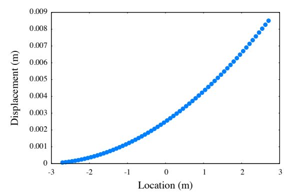
Partial-stress formulation



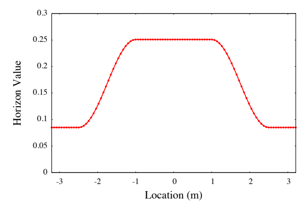
Patch Test: Prescribed Quadratic Displacement

Test set-up

Prescribe quadratic displacement field



Variable horizon

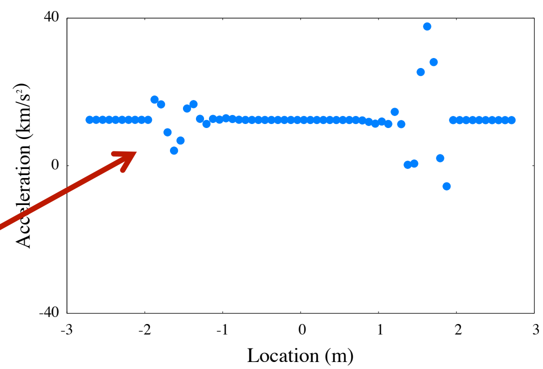


Can the standard model and the partial-stress model recover the expected constant acceleration?

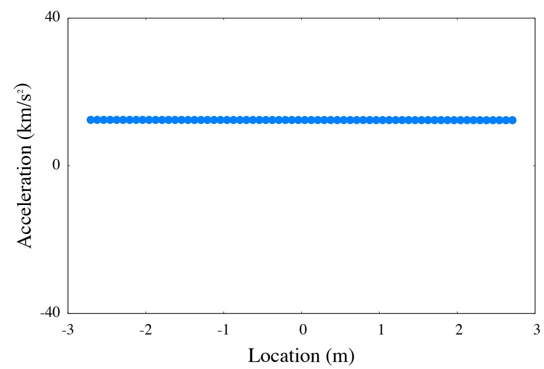
Only the **partial stress** formulation produce the expected result when the horizon is **varying**

Test Results: Acceleration over the length of the bar

Standard material model



Partial-stress formulation

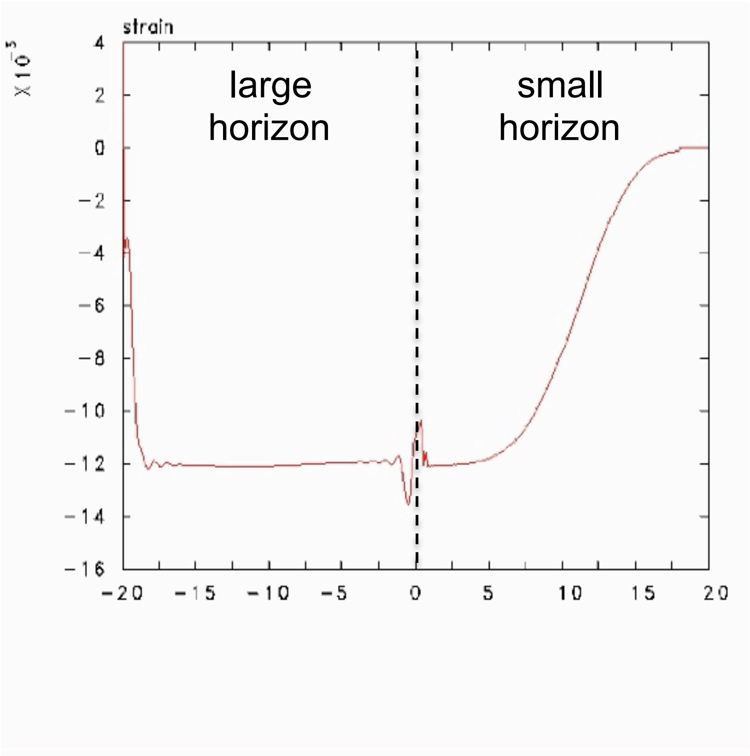


Spurious "ghost forces" present in standard formulation

Wave Propagation through Region of Varying Horizon

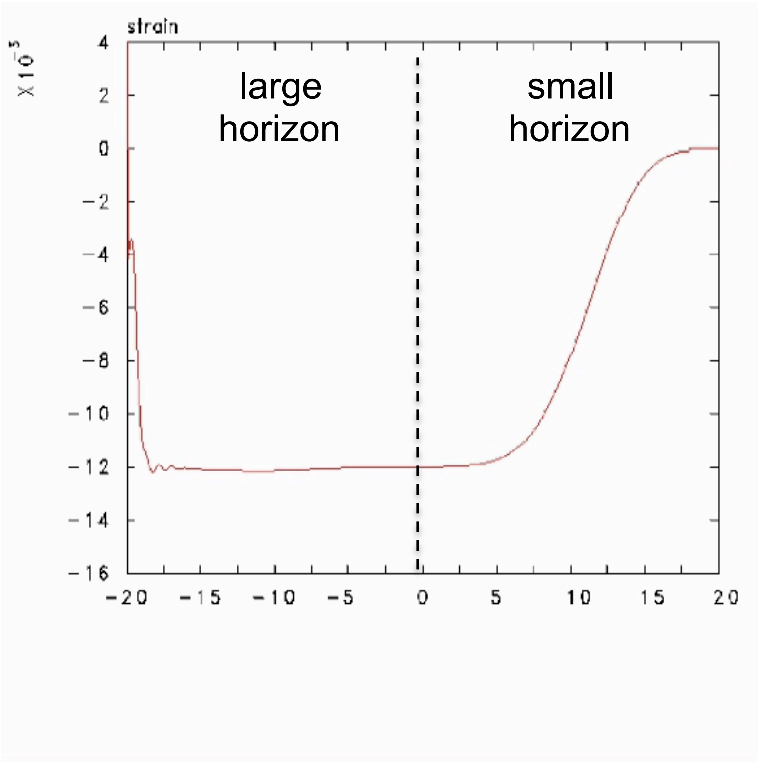
Standard peridynamic model

Numerical artifacts present at transition from large horizon to small horizon



Partial-stress approach

Greatly reduces artifacts, enables smooth transition between large and small horizons



[1] Silling, S., and Seleson, P., Variable Length Scale in a Peridynamic Body, SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, PA, June 12, 2013.

What about Performance?

USE OF A VARIABLE HORIZON IMPACTS PERFORMANCE IN SEVERAL WAYS

- Use of a variable horizon can reduce neighborhood size
  - Less computational cost per internal force evaluation
  - Reduces number of unknowns in stiffness matrix for implicit time integration
- Use of a variable horizon can reduce the critical time step
  - Critical time step is strongly dependent on the horizon [1, 2]
  - Smaller time step results in more total steps to solution for explicit transient dynamic simulations
  - Important note: the critical time step for analyses combining peridynamics and classical finite analysis is generally determine by the classical finite elements

Total Number of Bonds
(equal to number of nonzeros in stiffness matrix)

Constant Horizon	92.6 million
Varying Horizon	46.5 million

Stable Time Step [1, 2]
(explicit transient dynamics)

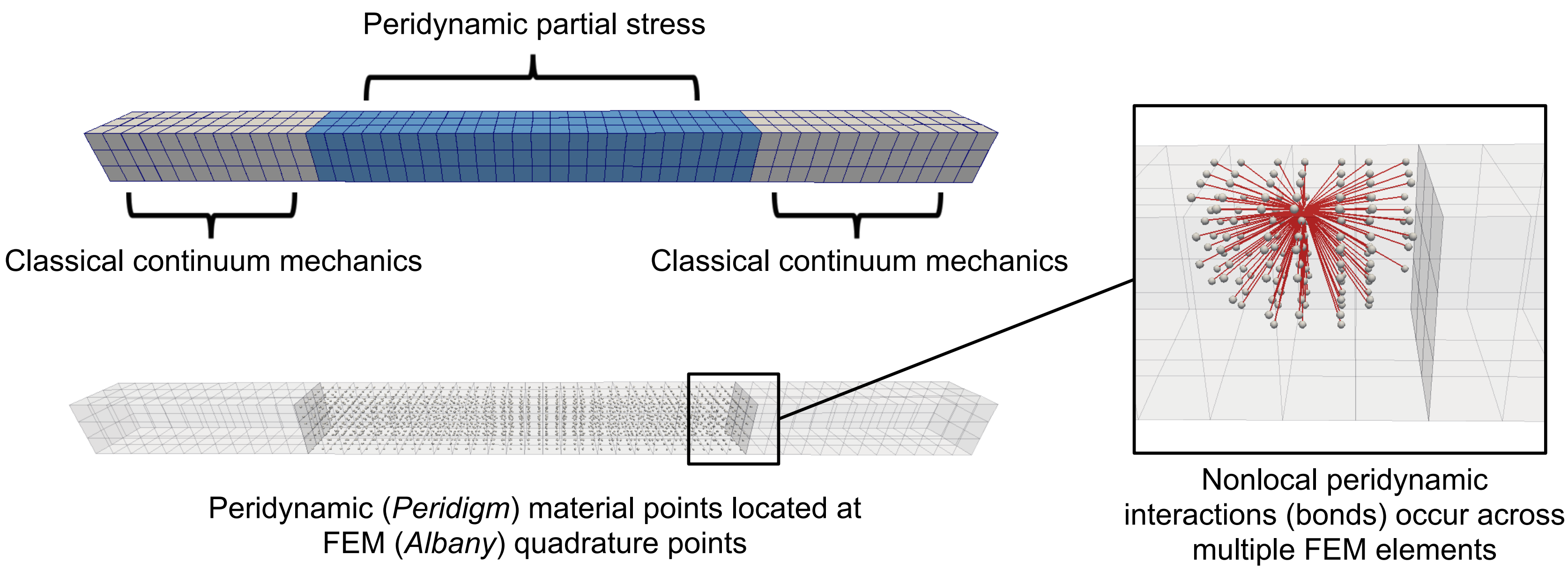
Constant Horizon	2.03e-5 sec.
Varying Horizon	7.15e-6 sec.

[1] S.A. Silling and E. Askari. A meshfree method based on the peridynamic model of solid mechanics. *Computers and Structures*, 83:1526-1535, 2005.

[2] Littlewood, D.J, Thomas, J.D., and Shelton, T.R. Estimation of the Critical Time Step for Peridynamic Models. SIAM Conference on the Mathematical Aspects of Material Science, Philadelphia, Pennsylvania, June 9-12, 2013.

A Prototype of the Partial Stress Formulation has been Implemented in Coupled *Albany-Peridigm* Code

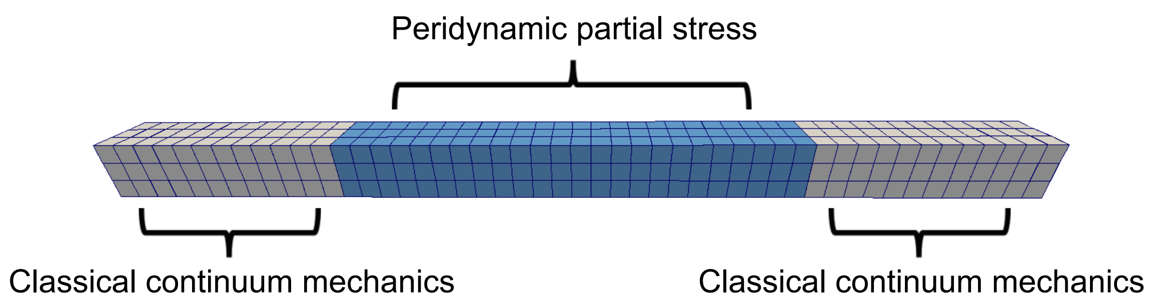
- Software infrastructure in place for strongly coupled simulations
- Meshfree peridynamic models, peridynamic partial stress, and classical continuum mechanics (FEM) within single executable
- Partial stress utilized for transition between classical continuum mechanics (local model) and peridynamics (nonlocal model)

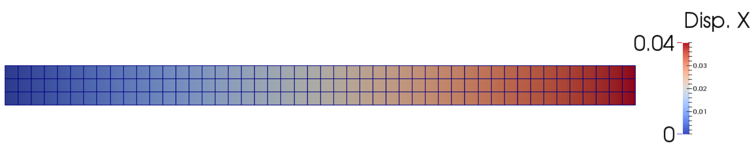


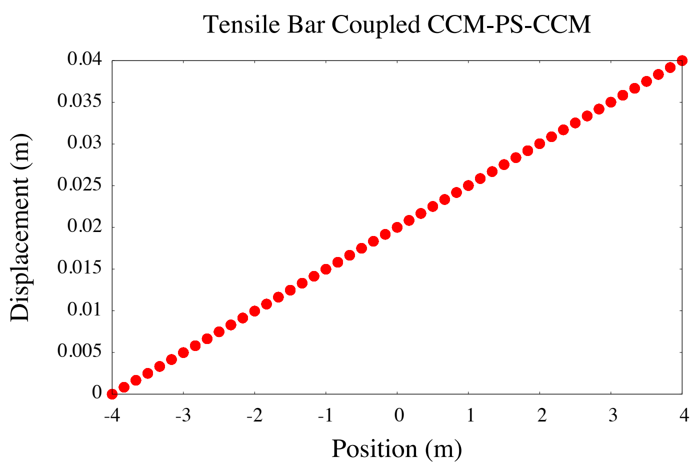
Demonstration Calculation

LINEAR PATCH TEST

- Coupling of classical continuum mechanics and peridynamic partial stress
- Local boundary conditions applied to areas at ends of bar (prescribed displacement)
- Implicit *Albany* solver (statics)



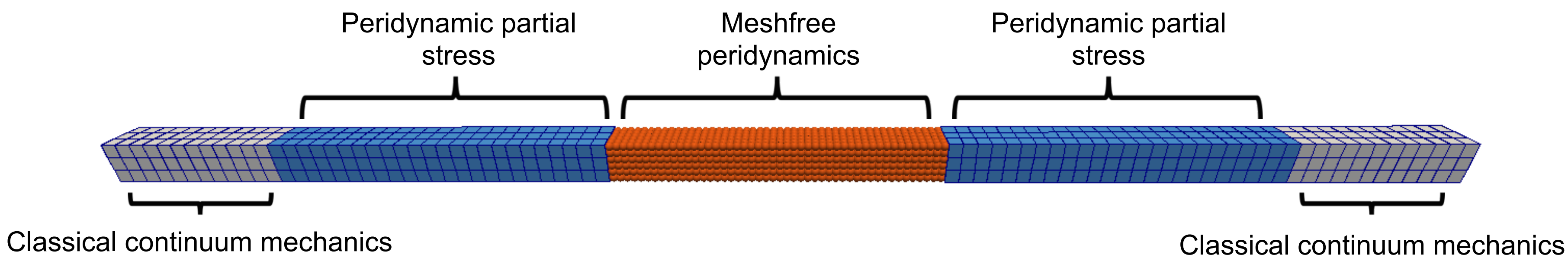


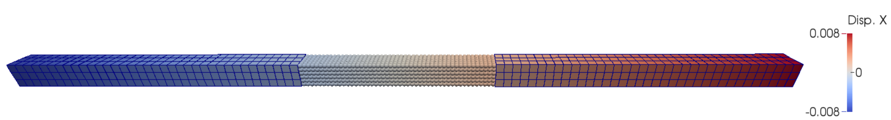


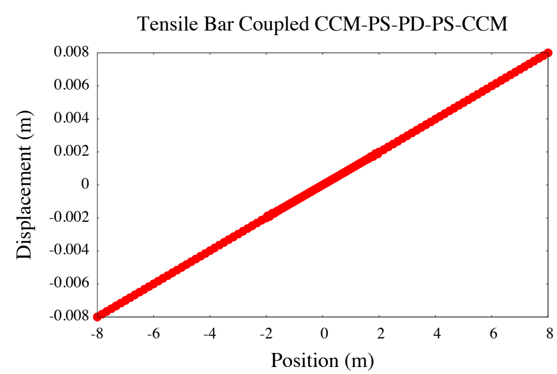
Demonstration Calculation

LINEAR PATCH TEST

- Coupling of classical continuum mechanics, peridynamic partial stress, and standard meshfree peridynamics
- Local boundary conditions applied to areas at ends of bar (prescribed displacement)
- Implicit *Albany* solver (statics)
- Interface between partial stress and meshfree peridynamics is a work in progress







Optimization-Based Local-Nonlocal Coupling

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CURRENT EFFORT OF D'ELIA, PEREGO, AND BOCHEV

- Model coupling can be cast as an optimization problem
- *Objective function*: Difference between solutions in overlap region
- *Constraints*: Governing equations of the individual models

APPLICATION OF OPTIMIZATION-BASED COUPLING TO COMPUTATIONAL SOLID MECHANICS

- Appropriate for static and quasi-static problems involving disparate models
- Rigorous mathematical foundation, error bounds, etc.
- Can be applied as a "black box" to couple dissimilar computational domains
- Computational expense is a concern, mitigation strategies being investigated

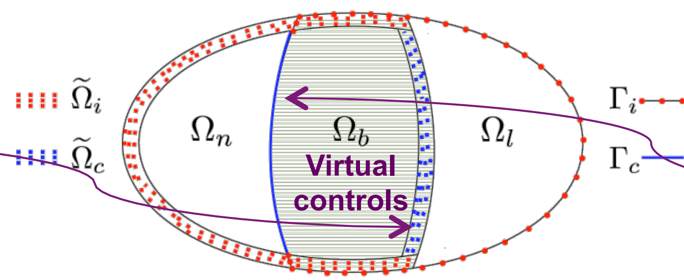
Optimization Based Coupling

Minimize the mismatch between the nonlocal and local models subject to the two models acting independently in Ω_N and Ω_L

$$\min_{u_n, u_l, \theta_n, \theta_l} J(u_n, u_l) = \frac{1}{2}\|u_n - u_l\|^2_{0,\Omega_b} \quad \text{s.t.}$$

Nonlocal

$$\begin{cases} -\mathcal{L}u_n = f_n & \boldsymbol{x} \in \Omega_n \\ u_n = \theta_n & \boldsymbol{x} \in \widetilde{\Omega}_c \\ u_n = 0 & \boldsymbol{x} \in \widetilde{\Omega}_i \end{cases}$$



Local

$$\begin{cases} -\Delta u_l = f_l & \boldsymbol{x} \in \Omega_l \\ u_l = \theta_l & \boldsymbol{x} \in \Gamma_c \\ u_l = 0 & \boldsymbol{x} \in \Gamma_i. \end{cases}$$

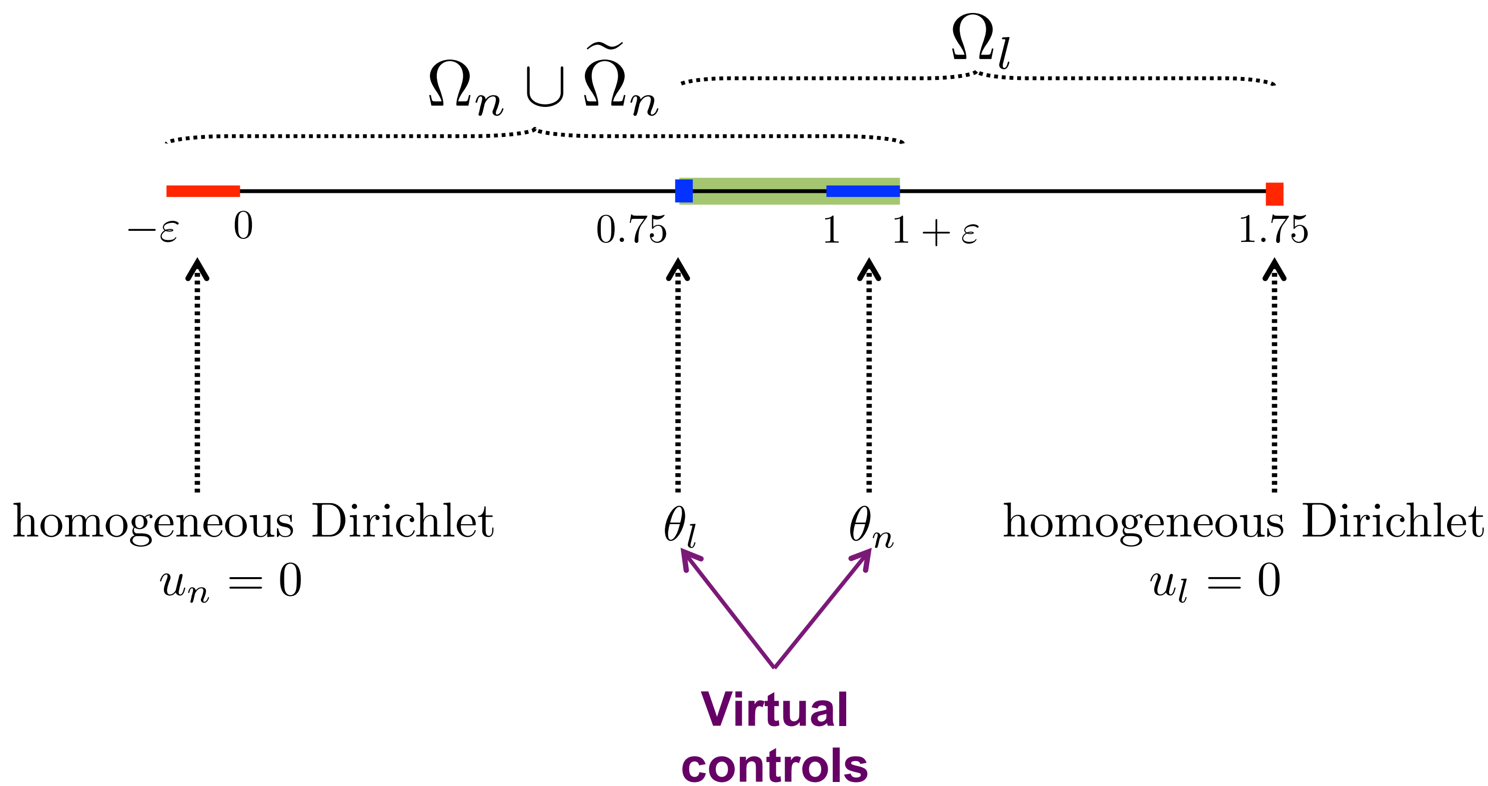
Key result of mathematical analysis:

Coupling error is bounded by the modeling error on the local subdomain

Slide material courtesy of D'Elia, Perego, and Bochev

Optimization-Based Coupling: Numerical Examples

PROBLEM SETTING IN 1D



Slide material courtesy of
D'Elia, Perego, and Bochev

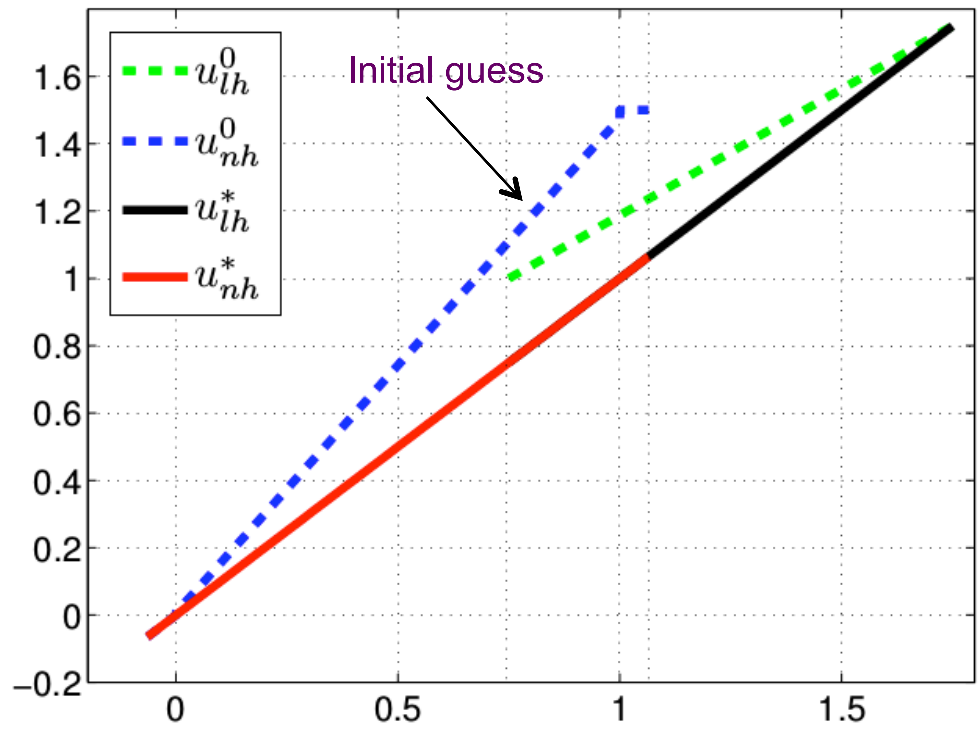
Optimization-Based Coupling: Numerical Examples

1D PATCH TEST

Kernel: $\gamma(x,y) = \dfrac{1}{\varepsilon^2 |x-y|} \chi(x-\varepsilon, x+\varepsilon)$

Exact solution:

- $u_n = u_l = x$
- $u_n|_{\widetilde{\Omega}_i} = x$
- $u_l(1.75) = 1.75$
- $f_n = f_l = 0$



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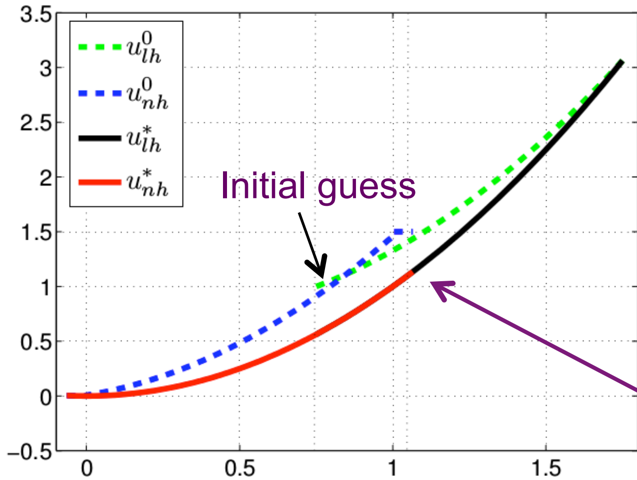
Optimization-Based Coupling: Numerical Examples

SMOOTH GLOBAL SOLUTION IN 1D

Example 1

- $u_n = u_l = x^2$
- $u_n|_{\widetilde{\Omega}_i} = x^2$
- $u_l(1.75) = 1.75^2$
- $f_n = f_l = -2$

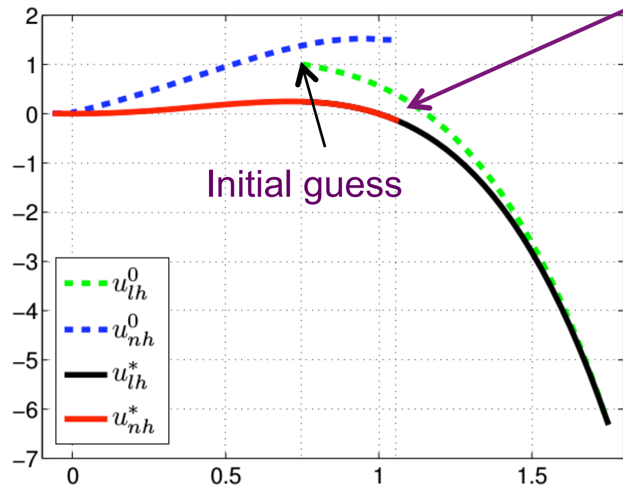


ε	h	$e(u_n)$	rate	$e(u_l)$	rate
0.065 test 1.	2^{-3}	2.36e-03	-	2.62e-03	-
	2^{-4}	7.54e-04	1.65	7.12e-04	1.88
	2^{-5}	1.88e-04	2.00	1.78e-04	2.00
	2^{-6}	4.67e-05	2.01	4.44e-05	2.00
	2^{-7}	1.14e-05	2.04	1.10e-05	2.01

Optimization approach merges the models seamlessly!

Example 2

- $u_n = u_l = x^2 - x^4$
- $u_n|_{\widetilde{\Omega}_i} = x^2 - x^4$
- $u_l(1.75) = 1.75^2 - 1.$
- $f_n = -2 + 12x^2 + \varepsilon^2$
- $f_l = -2 + 12x^2.$



ε	h	$e(u_n)$	rate	$e(u_l)$	rate
0.065 test 2.	2^{-3}	9.70e-03	-	2.95e-02	-
	2^{-4}	2.68e-03	1.86	7.54e-03	1.97
	2^{-5}	7.02e-04	1.93	1.90e-03	1.99
	2^{-6}	1.78e-04	1.98	4.76e-04	2.00
	2^{-7}	4.48e-05	1.99	1.19e-04	2.00

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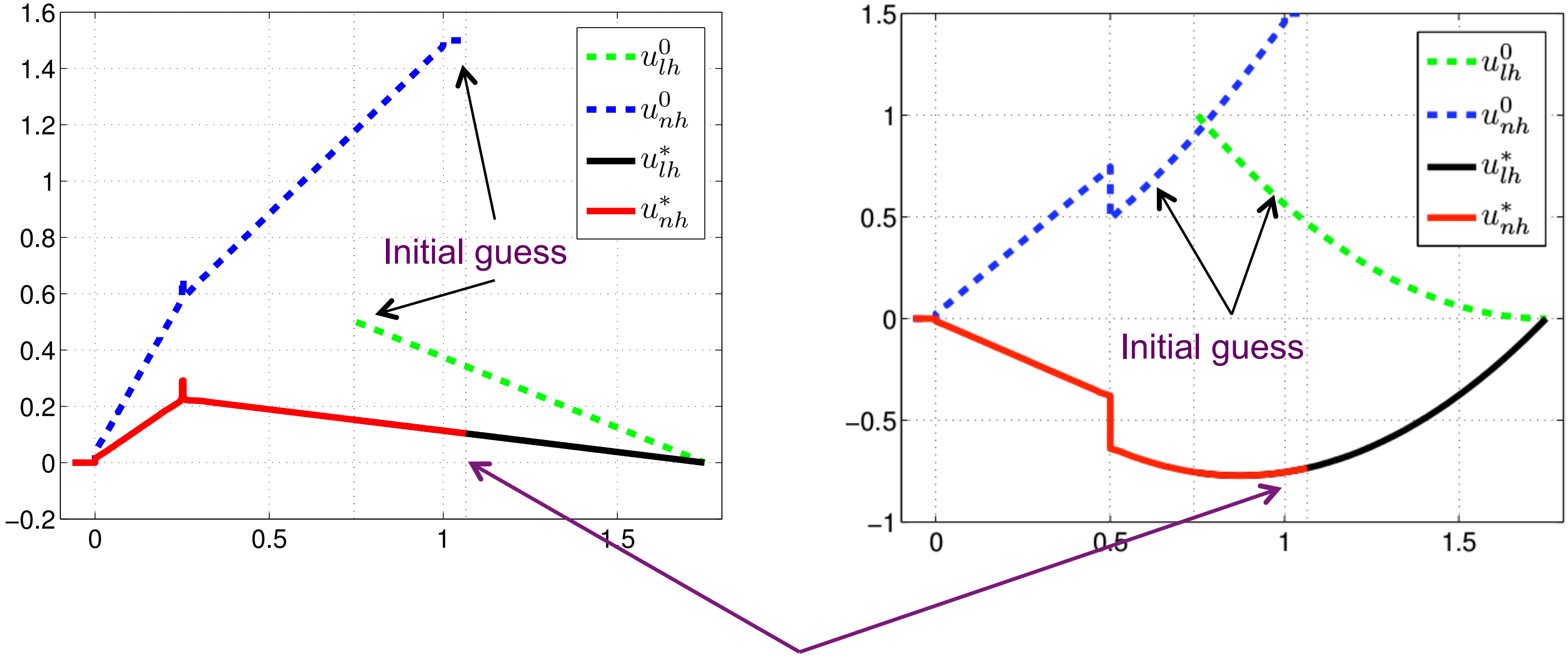
ROUGH NONLOCAL SOLUTION

Point force | **Discontinuous nonlocal state**



Optimization approach merges the models seamlessly!

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Optimization-Based Coupling: Path Forward

Research & proof-of-principle →  → **Programmatically exercised software**

Utilize agile components approach for development of computational algorithms

- Provide access to adjoints, sensitivites, etc. for adjoint-based fast optimization
- Enable effective transitioning of research ideas into production software

ROL →

$$\min_{u_n, u_l, \theta_n, \theta_l} J(u_n, u_l) \text{ s.t. } \begin{cases} -\mathcal{L}u_n = f_n & \boldsymbol{x} \in \Omega_n \\ u_n = \theta_n & \boldsymbol{x} \in \widetilde{\Omega}_c \\ u_n = 0 & \boldsymbol{x} \in \widetilde{\Omega}_i \end{cases} \quad \begin{cases} -\Delta u_l = f_l & \boldsymbol{x} \in \Omega_l \\ u_l = \theta_l & \boldsymbol{x} \in \Gamma_c \\ u_l = 0 & \boldsymbol{x} \in \Gamma_i. \end{cases}$$

Peridigm

Albany

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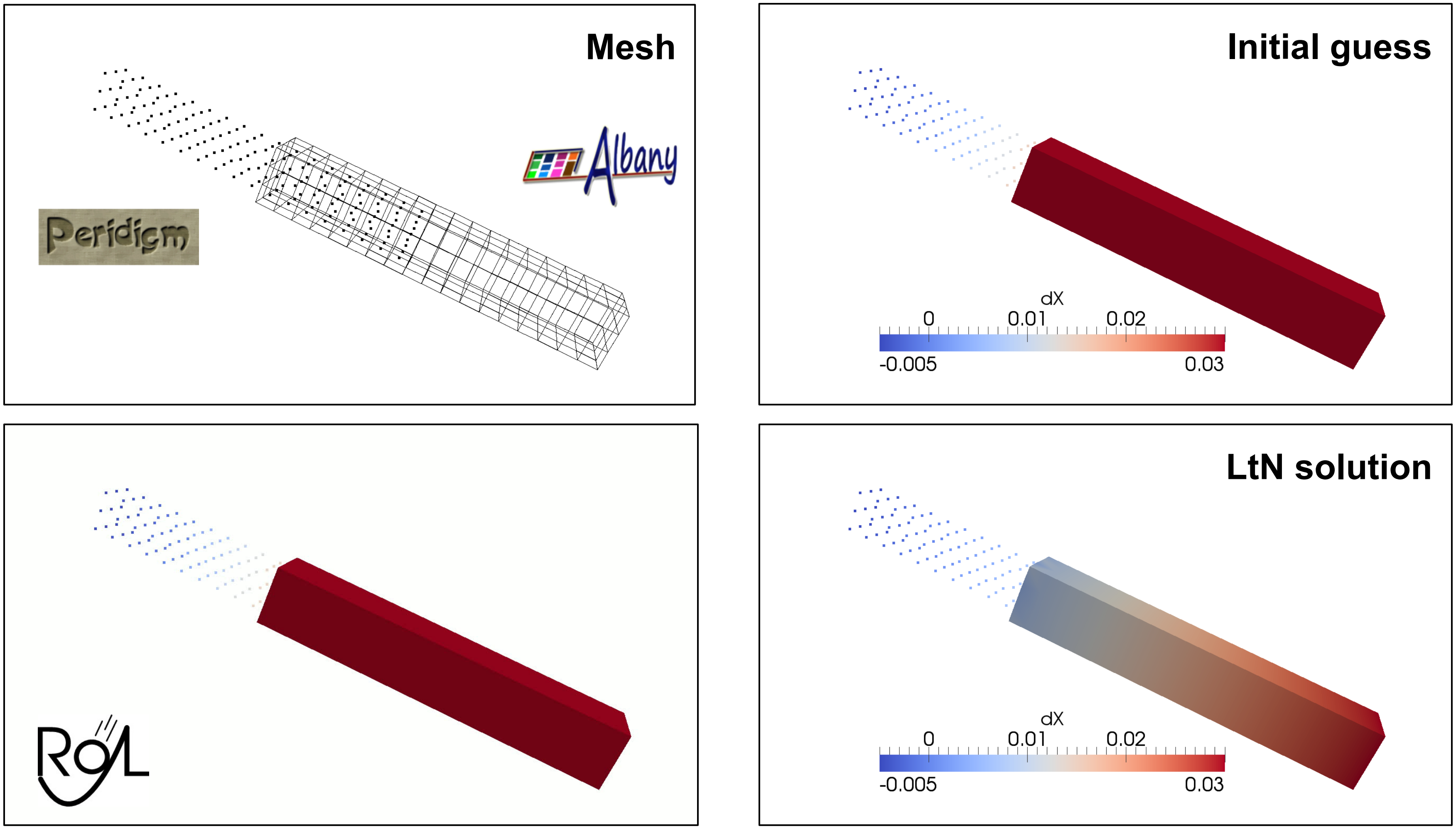
Optimization Based Coupling

PROOF-OF-CONCEPT SIMULATION COUPLING PERIDIGM AND ALBANY



Questions?

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Extra Slides

The *Peridigm* Computational Peridynamics Code

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WHAT IS PERIDIGM?

- Open-source software developed at Sandia National Laboratories
- C++ code based on Sandia's *Trilinos* project
- Platform for multi-physics peridynamic simulations
- Capabilities:
  - State-based constitutive models
  - Implicit and explicit time integration
  - Contact for transient dynamics
  - Large-scale parallel simulations
- Compatible with pre- and post-processing tools
  - Cubit mesh generation
  - Paraview visualization tools
  - SEACAS utilities
- Designed for extensibility

M.L. Parks, D.J. Littlewood, J.A. Mitchell, and S.A. Silling, Peridigm Users' Guide v1.0.0. Sandia Report SAND2012-7800, 2012.

Constitutive Models for Peridynamics

MATERIAL MODEL FORMULATION STRONGLY AFFECTS CRITICAL TIME STEP

- Presence of multiple length scales differs from the classical (local) approach
- Complex deformation modes possible within a nonlocal neighborhood
- Material failure through the breaking of bonds may alter the stable time step

Microelastic Material [1]

- Bond-based constitutive model
- Pairwise forces are a function of bond stretch

$$s = \frac{y - x}{x}$$

- Magnitude of pairwise force density given by

$$\underline{t} = \frac{18k}{\pi \delta^4} s$$

Linear Peridynamic Solid [2]

- State-based constitutive model
- Deformation decomposed into deviatoric and dilatational components

$$\theta = \frac{3}{m} \int_{\mathcal{H}} (\underline{\omega}\, \underline{x}) \cdot \underline{e}\, dV \qquad \underline{e}^d = \underline{e} - \frac{\theta\, \underline{x}}{3}$$

- Magnitude of pairwise force density given by

$$\underline{t} = \frac{3k\theta}{m} \underline{\omega}\, \underline{\mathrm{x}} + \frac{15\mu}{m} \underline{\omega}\, \underline{e}^{\mathrm{d}}$$

Definitions

$\underline{x}$	bond vector
x	initial bond length
y	deformed bond length
s	bond stretch
$\underline{e}$	bond extension
$\underline{e}^d$	deviatoric bond extension
$\underline{\omega}$	influence function
V	volume
$\mathcal{H}$	neighborhod
m	weighted volume
θ	dilatation
δ	horizon
k	bulk modulus
μ	shear modulus
$\underline{t}$	pairwise force density

1. S.A. Silling. Reformulation of elasticity theory for discontinuities and long-range forces. *Journal of the Mechanics and Physics of Solids*, 48:175-209, 2000.
2. S.A. Silling, M. Epton, O. Weckner, J. Xu, and E. Askari, Peridynamic states and constitutive modeling, *Journal of Elasticity*, 88, 2007.

Classical Material Models Can Be Applied in Peridynamics

WRAPPER APPROACH RESULTS IN A NON-ORDINARY STATE-BASED MATERIAL MODEL [1]

- Approximate deformation gradient based on initial and current locations of material points in family

Approximate Deformation Gradient

$$\bar{\mathbf{F}} = \left(\underline{\mathbf{Y}} * \underline{\mathbf{X}}\right) \mathbf{K}^{-1}$$

Shape Tensor

$$\mathbf{K} = \underline{\mathbf{X}} * \underline{\mathbf{X}}$$

Definitions

$\mathbf{X}$	reference position vector state
$\mathbf{Y}$	deformation vector state
$\mathbf{K}$	shape tensor
$\bar{\mathbf{F}}$	approximate deformation gradient
ξ	bond
$\underline{\omega}$	influence function
σ	Piola stress

- Kinematic data passed to classical material model
- Classical material model computes stress
- Stress converted to pairwise force density

$$\underline{\mathbf{T}} \left\langle \xi \right\rangle = \underline{\omega} \left\langle \xi \right\rangle \, \sigma \mathbf{K}^{-1} \xi$$

- Suppression of zero-energy modes (optional) [2]

1. S.A. Silling, M. Epton, O. Weckner, J. Xu, and E. Askari, Peridynamic states and constitutive modeling, *Journal of Elasticity*, 88, 2007.
2. Littlewood, D. A Nonlocal Approach to Modeling Crack Nucleation in AA 7075-T651. Proceedings of the ASME 2011 International Mechanical Engineering Congress and Exposition, Denver, Colorado, 2011.

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LOCAL AND NONLOCAL DIFFUSION MODELS

The nonlocal problem

$$\begin{cases} -\mathcal{L}u_n = f_n & \boldsymbol{x} \in \Omega \\ u_n = \sigma_n & \boldsymbol{x} \in \widetilde{\Omega}, \end{cases}$$

The nonlocal diffusion operator

$$\mathcal{L}u(\boldsymbol{x}) = \int_{\mathbb{R}^n} \big(u(\boldsymbol{y}) - u(\boldsymbol{x})\big)\,\gamma(\boldsymbol{x},\boldsymbol{y})\,d\boldsymbol{y}$$

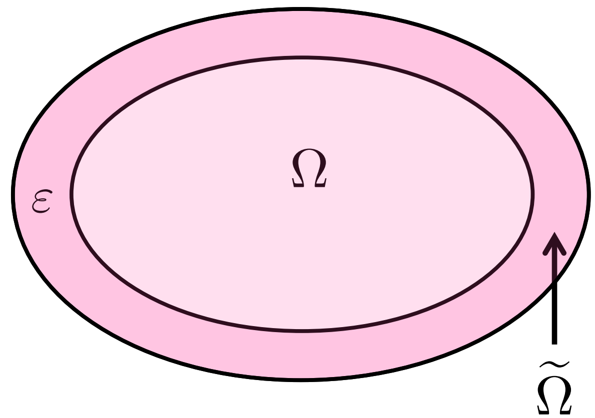
acting on $u(\boldsymbol{x})\colon \mathbb{R}^d \to \mathbb{R}$

The local problem

local diffusion model given by the Poisson equation

$$\begin{cases} -\Delta u_l = f_l & \boldsymbol{x} \in \Omega \\ u_l = \sigma_l & \boldsymbol{x} \in \partial\Omega, \end{cases}$$

where $\sigma_l \in H^{\frac{1}{2}}(\partial\Omega)$ and $f_l \in L^2(\Omega)$



D'Elia, M. and Bochev, P. Materials Research Society. Cambridge University Press, 2015.

D'Elia, M. and Bochev, P., *Submitted* 2015.