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Optimization-Based Coupling for Local and Nonlocal Models

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Center for Computing Research

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Model Coupling as an Optimization Problem

Goal: Simulation capability that combines disparate models

- Restrict use of high-fidelity models to subdomains to reduce overall cost
- Utilize multiscale and/or multiphysics models only where needed
- Overcome challenges resulting from disparate discretization strategies

Challenge: Inherent mismatch at model interface

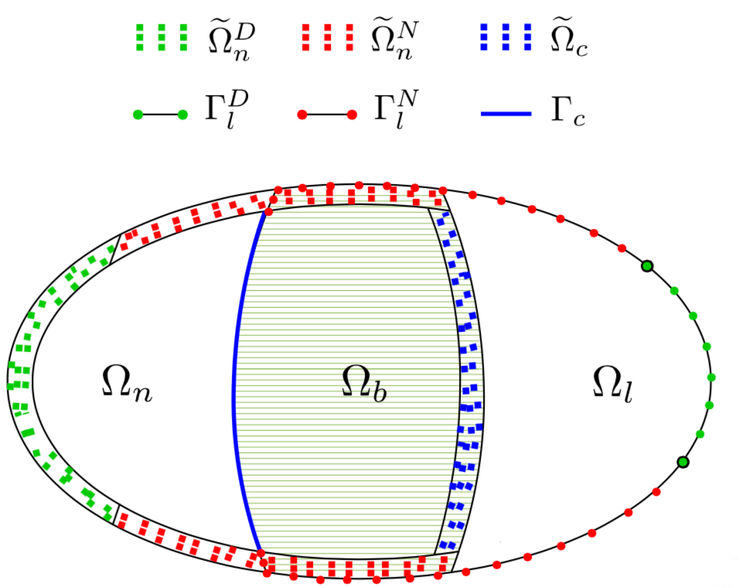
- Fundamentally different mathematical models
- Discretization schemes that are not directly compatible
- Disparate physics and/or length scales

Approach: Cast model coupling as an optimization problem

- Minimize difference between solutions in overlap region
- Governing equations of the individual models act as constraints
- Roles of coupling conditions and models are reversed with respect to standard coupling methods

Optimization Based Local-Nonlocal Coupling

Minimize the mismatch between local and nonlocal models subject to the two models acting independently in their respective domains



$$\min_{u_n,u_l,\theta_n,\theta_l} J(u_n,u_l) = \frac{1}{2}\int_{\Omega_b}(u_n-u_l)^2\,d\boldsymbol{x} = \frac{1}{2}\|u_n-u_l\|^2_{0,\Omega_b}$$

subject to

<u>Nonlocal model</u>

$$\begin{aligned} -\mathcal{L}u_n &= f_n & \boldsymbol{x}\in\Omega_n \\ u_n &= \theta_n & \boldsymbol{x}\in\widetilde{\Omega}_c \\ u_n &= 0 & \boldsymbol{x}\in\Omega_n^D \\ -\mathcal{N}(\mathcal{G}u_n) &= 0 & \boldsymbol{x}\in\widetilde{\Omega}_n^N \end{aligned}$$

<u>Local model</u>

$$\begin{aligned} -\Delta u_l &= f_l & \boldsymbol{x}\in\Omega_l \\ u_l &= \theta_l & \boldsymbol{x}\in\Gamma_c \\ u_l &= 0 & \boldsymbol{x}\in\Gamma_l^D \\ \nabla u_l\cdot\mathbf{n} &= 0 & \boldsymbol{x}\in\Gamma_l^N \end{aligned}$$

where the nonlocal operators are defined as [Du, et al., 2013]:

$$\mathcal{L}u(\boldsymbol{x}) = 2\int_{\mathbb{R}^d}\big(u(\boldsymbol{y})-u(\boldsymbol{x})\big)\,\gamma(\boldsymbol{x},\boldsymbol{y})\,d\boldsymbol{y} \quad \boldsymbol{x}\in\mathbb{R}^d$$

$$\mathcal{N}(\boldsymbol{\nu})(\boldsymbol{x}) = -\int_{\Omega^+}(\boldsymbol{\nu}(\boldsymbol{x},\boldsymbol{y})+\boldsymbol{\nu}(\boldsymbol{y},\boldsymbol{x}))\,\boldsymbol{\alpha}(\boldsymbol{x},\boldsymbol{y})\,d\boldsymbol{y} \quad \boldsymbol{x}\in\widetilde{\Omega}$$

$$\mathcal{G}(u)(\boldsymbol{x},\boldsymbol{y}) := \big(u(\boldsymbol{y})-u(\boldsymbol{x})\big)\boldsymbol{\alpha}(\boldsymbol{x},\boldsymbol{y}) \quad \boldsymbol{x},\boldsymbol{y}\in\mathbb{R}^d$$

Analysis has established existence, uniqueness of solution to coupled problem

D'Elia, M., Perego, M., Bochev, P., and Littlewood, D. A coupling strategy for nonlocal and local diffusion models with mixed volume constraints and boundary conditions. *Computers and Mathematics with Applications* 71, 2218-2230, 2016.

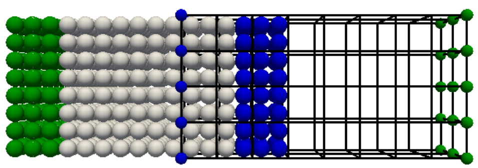
Du, Q., Gunzburger, M., Lehoucq, R.B., and Zhou, K. A nonlocal vector calculus, nonlocal volume-constrained problems, and nonlocal balance laws, *Mathematical Models and Methods in Applied Sciences* 23(03), 493-540, 2013.

Example: Coupling of Local and Nonlocal Diffusion Models

Recovery of linear solution using coupled local-nonlocal model

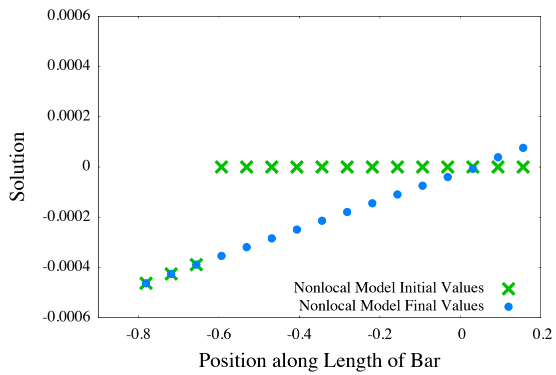
- Boundary conditions applied to ends of bar
  - Linear solution imposed over volumetric region of nonlocal model
  - Standard local boundary conditions applied to local model
- Optimization-based approach successfully couples local and nonlocal models

Problem Set-up

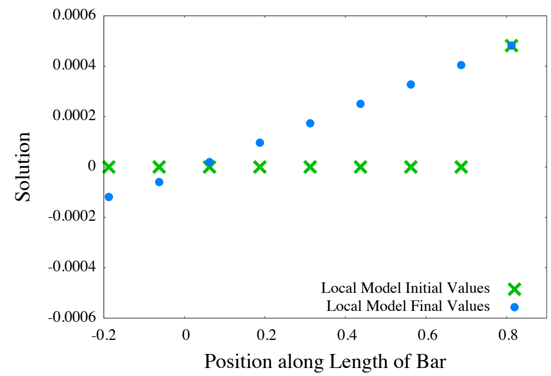


Coupled solution

Solution of local model



Solution of nonlocal model

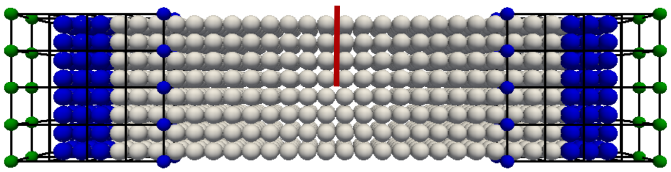


Example: Local and Nonlocal Diffusion in a Pre-Cracked Bar

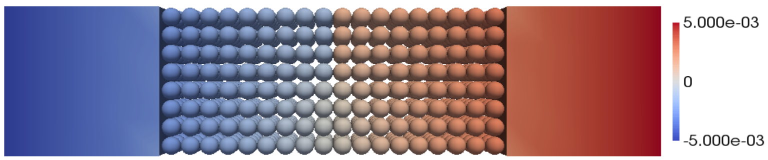
Local boundary conditions applied to pre-cracked bar

- Boundary conditions applied to local model only
  - Avoids difficulties in applying volume constraints to nonlocal model
- Optimization-based approach successfully couples local and nonlocal models
- Nonlocal model provides solution in vicinity of crack

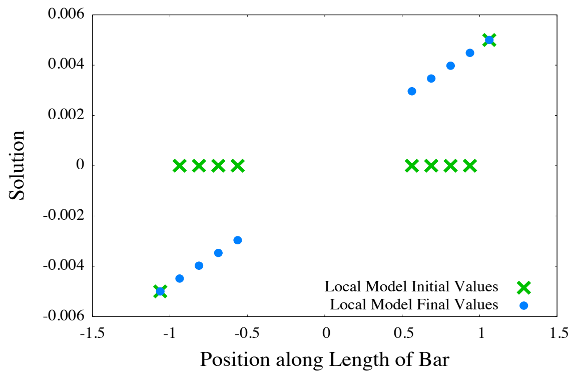
Problem Set-up



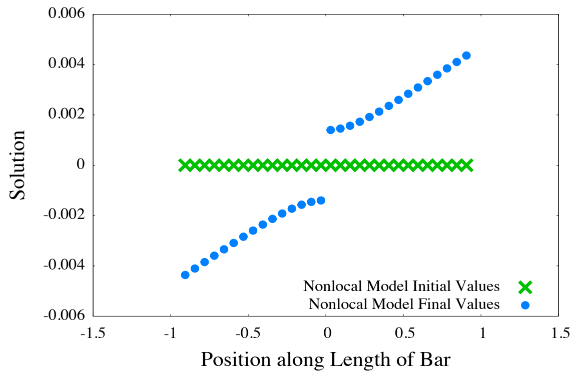
Coupled solution



Solution of local model along top of bar



Solution of nonlocal model along top of bar



Optimization-Based Coupling for Local and Nonlocal Elasticity

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Extension of the optimization-based coupling approach of D'Elia, et al., to local-nonlocal coupling for 3D elasticity

- Classical (local) elasticity model provided by *Albany/LCM* code
- Peridynamic (nonlocal) elasticity model provided by *Peridigm* code
- *Rapid Optimization Library (ROL)* utilized for minimization of functional

ROL

$$\min_{\mathbf{u}_n,\mathbf{u}_l,\boldsymbol{\nu}_n,\boldsymbol{\nu}_l} \mathcal{J}(\mathbf{u}_n,\mathbf{u}_l) = \frac{1}{2}\int_{\Omega_o} \|\mathbf{u}_n - \mathbf{u}_l\|_{\ell_2}^2 \, d\mathbf{x}$$

s.t.

$$\begin{cases} -\mathcal{L}_{\mathrm{LPS}}[\mathbf{u}_n](\mathbf{x}) = \mathbf{b}(\mathbf{x}) & \mathbf{x} \in \omega_n \\ \mathbf{u}_n(\mathbf{x}) = \mathbf{g}(\mathbf{x}) & \mathbf{x} \in \eta_D \\ \mathbf{u}_n(\mathbf{x}) = \boldsymbol{\nu}_n(\mathbf{x}) & \mathbf{x} \in \eta_c \end{cases}$$

Peridigm

$$\begin{cases} -\mathcal{L}_{\mathrm{NC}}[\mathbf{u}_l](\mathbf{x}) = \mathbf{b}(\mathbf{x}) & \mathbf{x} \in \Omega_l \\ \mathbf{u}_l(\mathbf{x}) = \mathbf{g}(\mathbf{x}) & \mathbf{x} \in \Gamma_D \\ \mathbf{u}_l(\mathbf{x}) = \boldsymbol{\nu}_l(\mathbf{x}) & \mathbf{x} \in \Gamma_c \end{cases}$$

Albany

$\boldsymbol{\nu}_n(\mathbf{x}), \boldsymbol{\nu}_l(\mathbf{x})$: control variables

Local and Nonlocal Elasticity Models

Nonlocal model

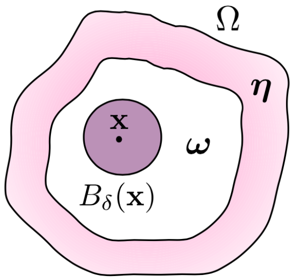
- Peridynamic model of solid mechanics with linearized Linear Peridynamic Solid (LPS) constitutive model
- Strong form solved using the meshless method of Silling and Askari

$$-\mathcal{L}_{\mathrm{LPS}}[\mathbf{u}](\mathbf{x}) = \mathbf{b}(\mathbf{x}), \quad \mathbf{x} \in \omega \text{ with constraints in } \eta$$

$$\mathcal{L}_{\mathrm{LPS}}[\mathbf{u}](\mathbf{x}) = \int_{\Omega \cap B_\delta(\mathbf{x})} \{\mathbf{T}[\mathbf{x}]\langle \mathbf{x}' - \mathbf{x}\rangle - \mathbf{T}[\mathbf{x}']\langle \mathbf{x} - \mathbf{x}'\rangle\}\, dV'_{\mathbf{x}}$$

$$B_\delta(\mathbf{x}) = \{\mathbf{x}' \in \mathbb{R}^d : \|\mathbf{x} - \mathbf{x}'\| \leq \delta\}$$

$$\mathbf{T}[\mathbf{x}]\langle \boldsymbol{\xi}\rangle = \tfrac{3K-5G}{m}\, \omega(\|\boldsymbol{\xi}\|)\, \theta(\mathbf{x})\boldsymbol{\xi} + \tfrac{15G}{m}\, \omega(\|\boldsymbol{\xi}\|)\, \tfrac{\boldsymbol{\xi}\otimes\boldsymbol{\xi}}{\|\boldsymbol{\xi}\|}(\mathbf{u}(\mathbf{x}+\boldsymbol{\xi}) - \mathbf{u}(\mathbf{x}))$$



bounded body $\Omega = \omega \cup \eta$
ω: domain
η: interaction domain
δ: interaction radius

Local model

- Navier-Cauchy equations of classical elasticity
- Standard finite element approach applied to solve the variational form

$$-\mathcal{L}_{\mathrm{NC}}[\mathbf{u}](\mathbf{x}) = \mathbf{b}(\mathbf{x}), \quad \mathbf{x} \in \Omega \text{ with conditions on } \partial\Omega$$

$$\mathcal{L}_{\mathrm{NC}}[\mathbf{u}](\mathbf{x}) := \left[\left(K + \tfrac{1}{3}G\right)\nabla(\nabla\cdot\mathbf{u})(\mathbf{x}) + G\,\nabla^2\mathbf{u}(\mathbf{x})\right]$$

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

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

Silling, S.A. Linearized theory of peridynamic states, *Journal of Elasticity* 99, 85-1111, 2010.

3D Elasticity: Linear Patch Test

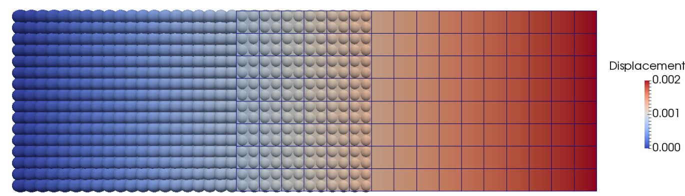
Recovery of linear solution using coupled local-nonlocal model

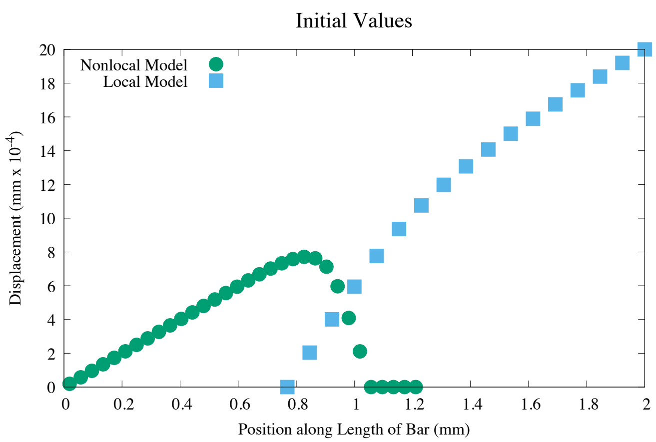
- Constraints applied at all free surfaces
  - Linear solution imposed over volumetric regions of nonlocal model
  - Standard local boundary conditions applied to surfaces of local model
- Optimization-based approach successfully recovers analytic solution (linear)

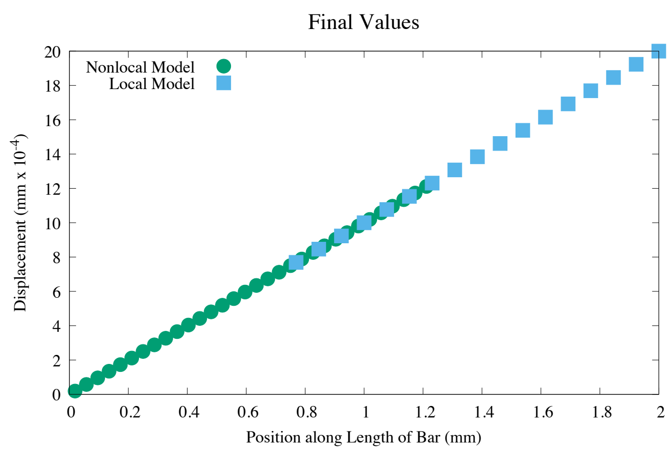
Model Parameters

Bulk modulus	160.0 GPa
Shear modulus	96.0 GPa
Horizon	0.0541 L

L = length of bar







Seleson, P., and Littlewood, D. Convergence studies in meshfree peridynamic simulations, Computers and Mathematics with Applications 71, 2432-2448, 2016.

3D Elasticity: Quadratic Patch Test

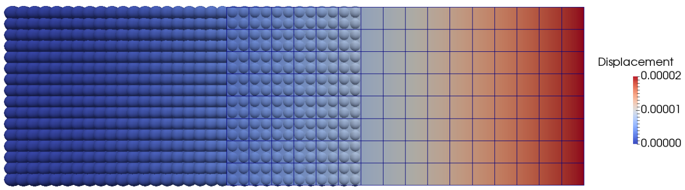
Recovery of quadratic solution using coupled local-nonlocal model

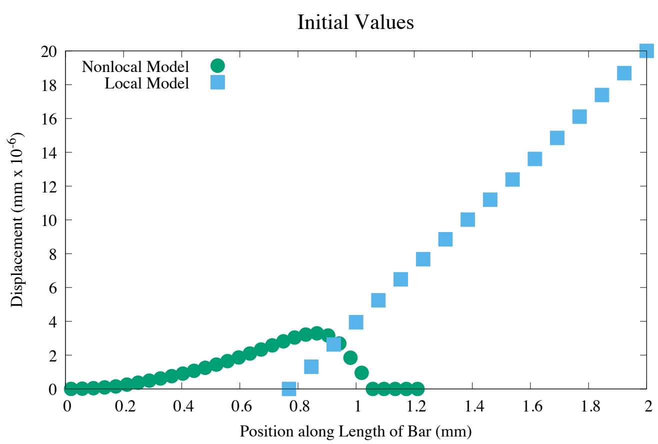
- Boundary conditions / nonlocal constraints
  - Linear solution imposed over volumetric regions of nonlocal model
  - Standard local boundary conditions applied to surfaces of local model
  - Body force applied to internal domains
- Optimization-based approach successfully recovers analytic solution (quadratic)

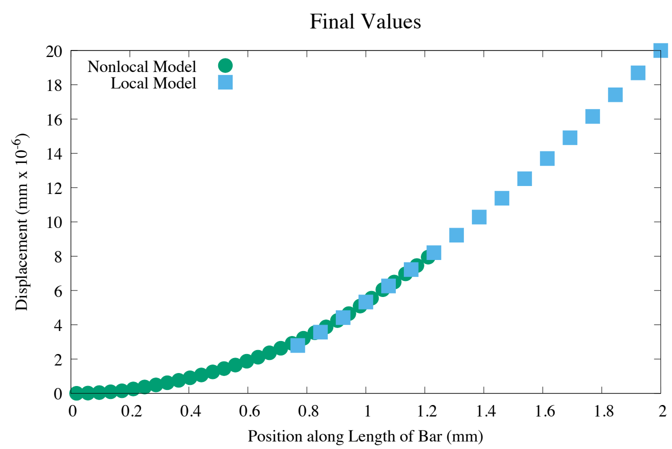
Model Parameters

Bulk modulus	160.0 GPa
Shear modulus	96.0 GPa
Horizon	0.0541 L

L = length of bar





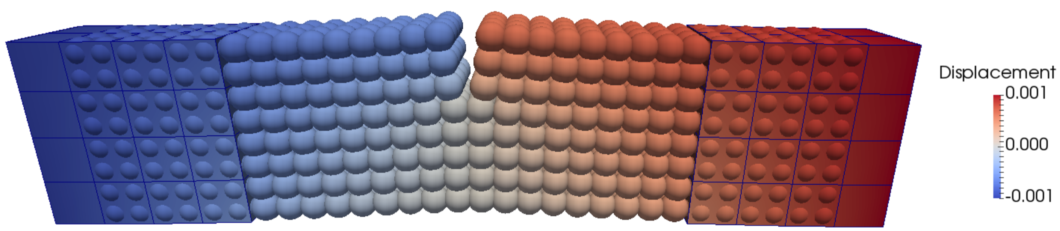


Seleson, P., and Littlewood, D. Convergence studies in meshfree peridynamic simulations, Computers and Mathematics with Applications 71, 2432-2448, 2016.

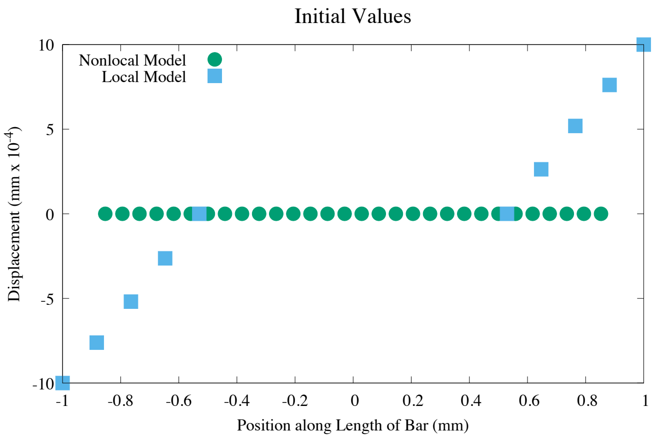
Bar with Pre-Crack Loaded in Tension

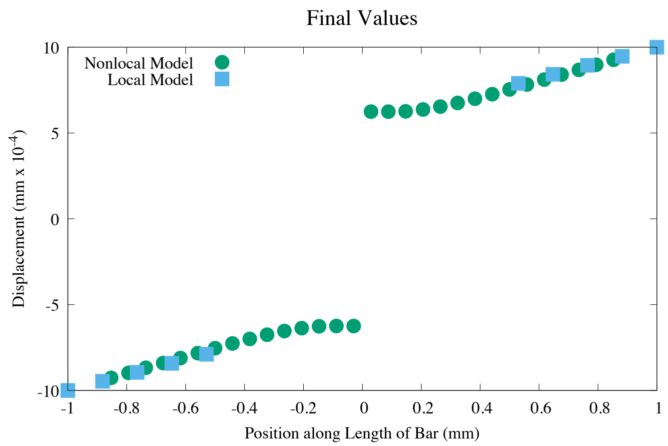
Combination of local and nonlocal models for "best of both worlds"

- Boundary conditions applied only to local model
  - Simple and well understood
- Peridynamic model applied in vicinity of crack
  - Nonlocal model is best suited to model crack region



Displacements magnified 50x for visualization purposes

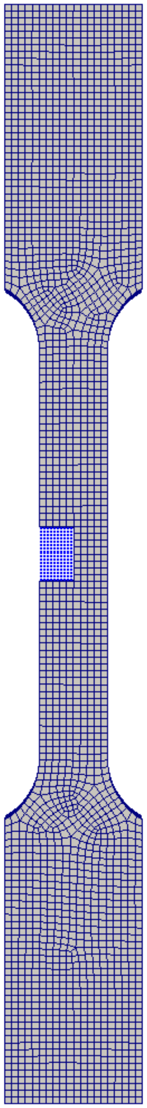




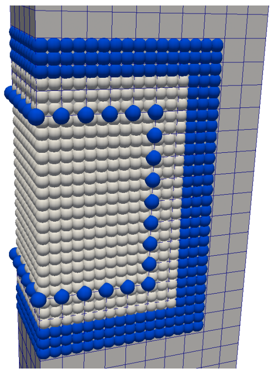
Tension Test

Application of coupling strategy to realistic geometry

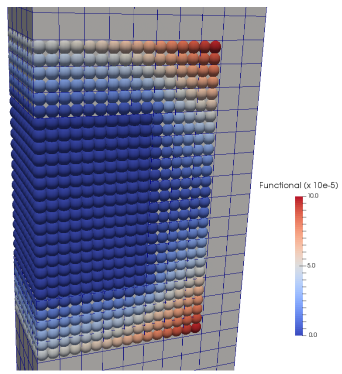
- Boundary conditions applied only to local model
- Peridynamic model restricted to small subdomain



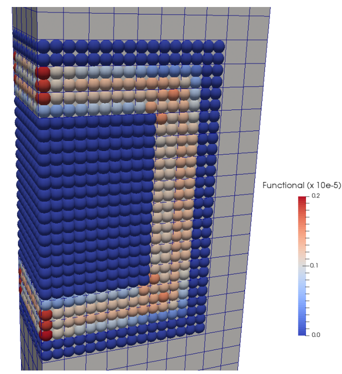
Control nodes



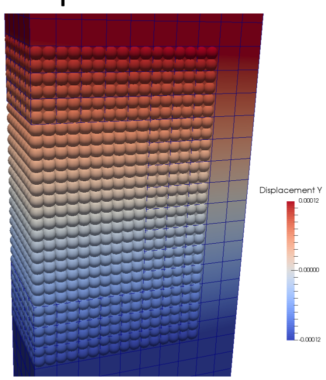
Initial functional values
J = 1.41e-2



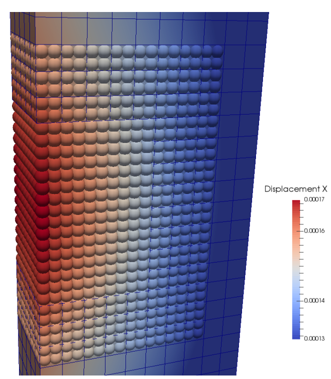
Final functional values
J = 4.31e-6



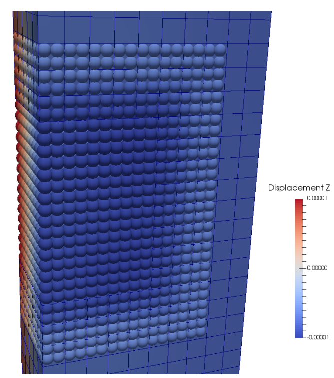
Displacement Y



Displacement X



Displacement Z



Influence of peridynamic surface effect

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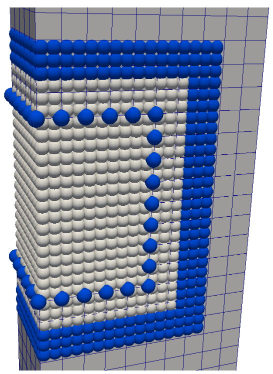
Tension Test with Pre-Crack

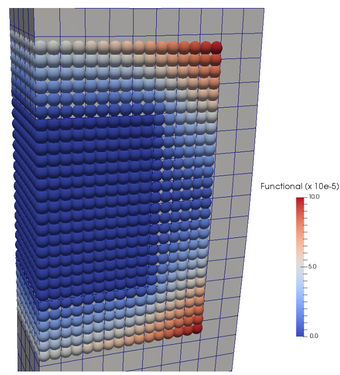
Application of coupling strategy to realistic geometry

- Boundary conditions applied only to local model
- Peridynamic model restricted to small subdomain

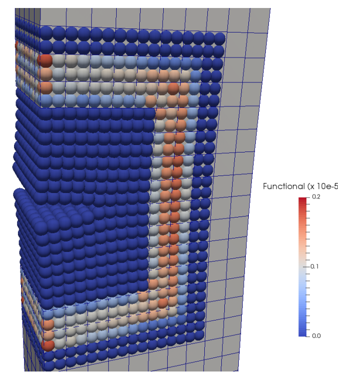
Control nodes



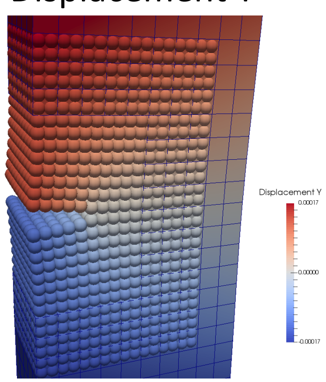
Initial functional values
J = 1.41e-2



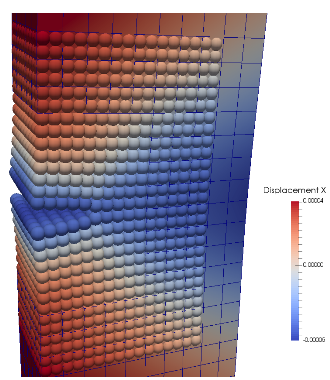
Final functional values
J = 3.80e-6



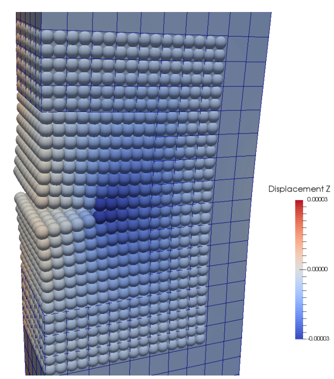
Displacement Y



Displacement X



Displacement Z



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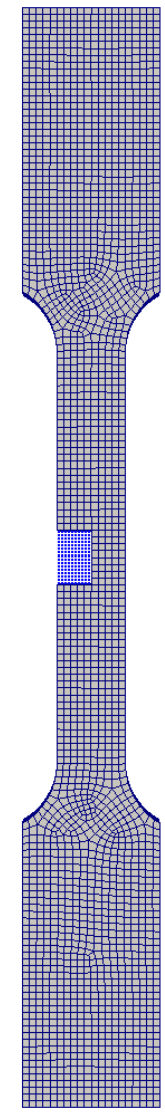

Ongoing Work

Improvements to optimization-based local-nonlocal coupling strategy

- Improvements in computational efficiency
  - Initial guess for solution on control nodes (utilize fully-local solution?)
  - Obtain second derivative information analytically (i.e., without finite difference) for use with ROL optimization routines
- Quasi-statics
- Crack growth
- Explicit dynamics

Questions?

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https://peridigm.sandia.gov

https://github.com/gahansen/albany