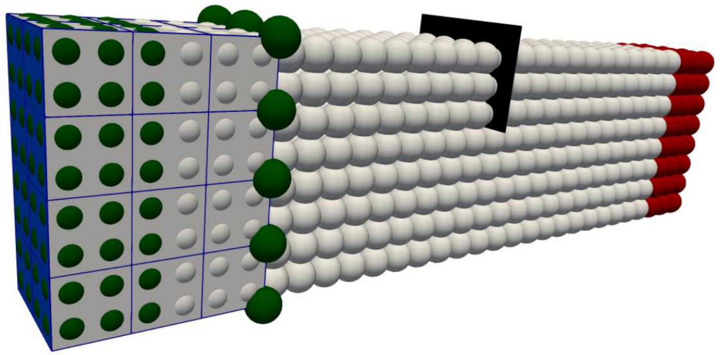
OPTIMIZATION-BASED APPROACHES

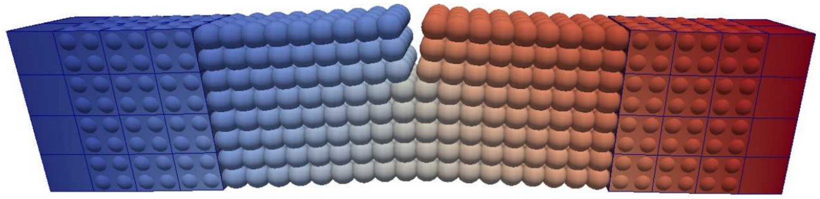
SAND2018-9302C

FOR IMPROVING EFFICIENCY AND ACCURACY OF NONLOCAL MECHANICS SIMULATIONS

Marta D'Elia, Center for Computing Research, SNL

LAWOC, Quito, Ecuador, September 3–7, 2018





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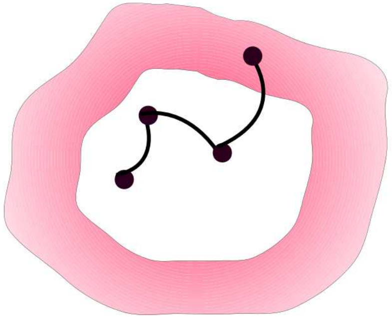
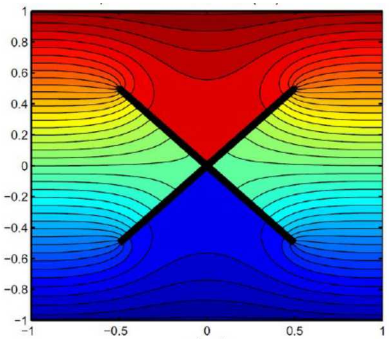
INTRODUCTION AND MOTIVATION

NOT ONLY MECHANICS…



- nonlocal models for continuum mechanics
- stochastic jump processes
- nonlocal heat conduction
- subsurface flow/porous media
- image processing

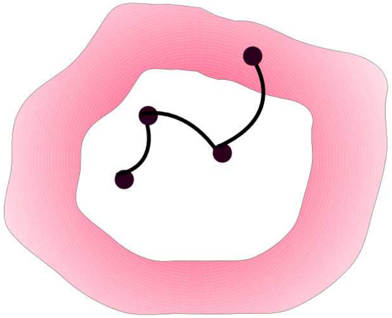
Wikipedia



Bobaru, 2012

Buades, 2010

NOT ONLY MECHANICS...



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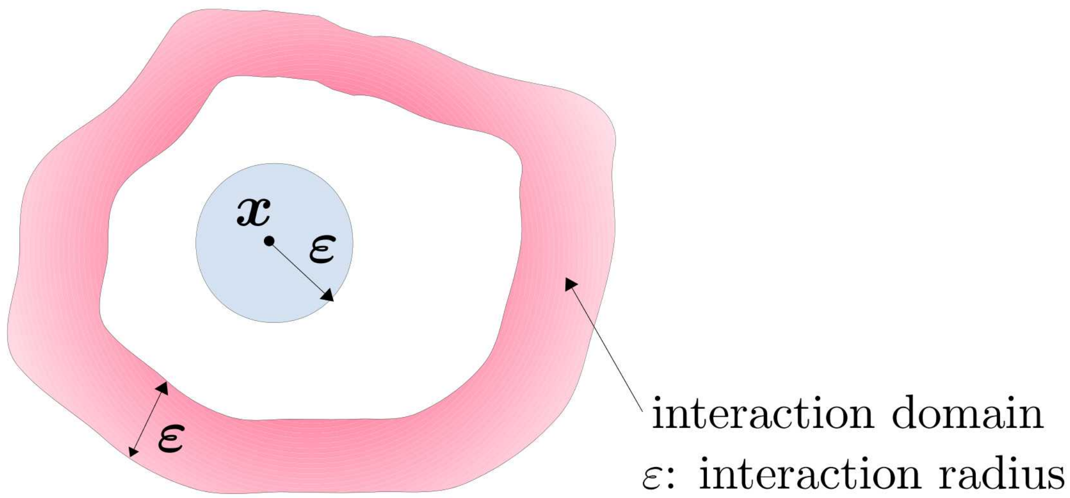
applicability: nonlocal diffusion operators

$$\mathcal{L}u(\boldsymbol{x}) = \int \big(u(\boldsymbol{y}) - u(\boldsymbol{x})\big)\, \gamma(\boldsymbol{x}, \boldsymbol{y})\, d\boldsymbol{y}$$

(...or more complex operators, more later)

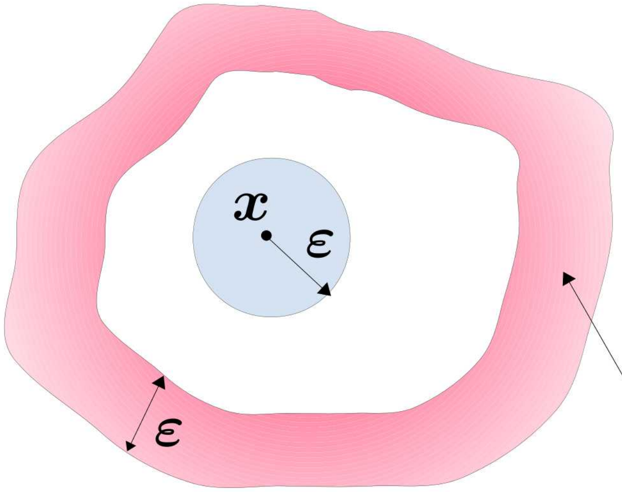
MECHANICS

- interactions can occur at distance, without contact



MECHANICS

- interactions can occur at distance, without contact
- used in many scientific and engineering applications, where the material dynamics depends on microstructure
- example: nonlocal continuum mechanics theories, e.g. **peridynamics** and physics-based **nonlocal elasticity** which can model fractures and material failures
- nonlocal models accurately resolve **small scale features**, e.g. dislocations



interaction domain
ε: interaction radius

MECHANICS

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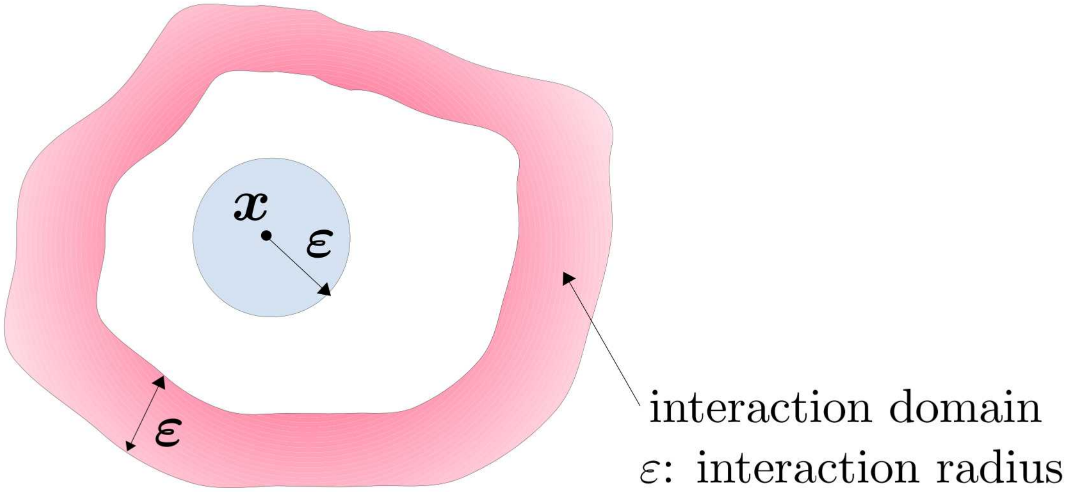

facts:

- a recently developed theoretical and numerical analysis allows us to study nonlocal problems **similarly** to the local (classical) counterpart

- we have **numerical convergence** results for finite element approximations

MECHANICS

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- we have **numerical convergence** results for finite element approximations

challenges: accuracy comes at a price!

- the numerical solution might be **prohibitively expensive**
- prescription of nonlocal "boundary conditions" is not straightforward

COUPLING

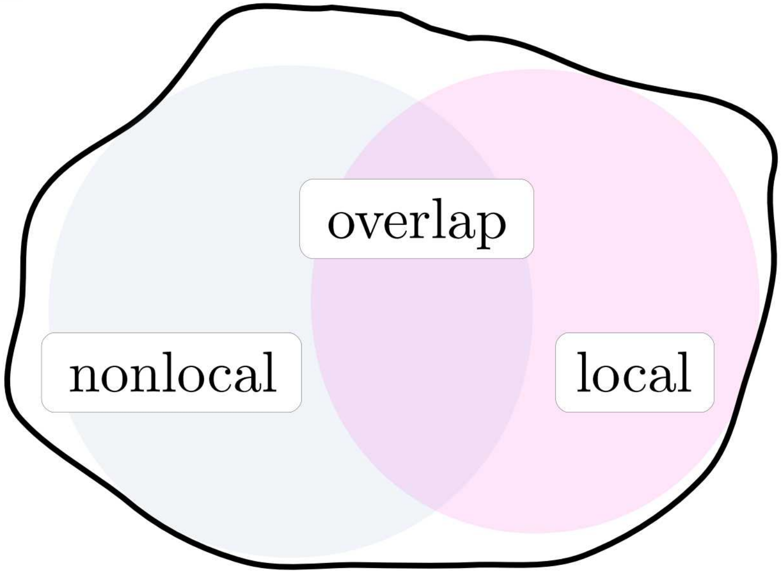
"Whenever you can use a local model, do it", Q. Du

– M. D'Elia, M. Perego, P. Bochev, D. Littlewood, A coupling strategy for local and nonlocal diffusion models with mixed volume constraints and boundary conditions, *Computers and Mathematics with applications*, 2015

– M. D'Elia, P. Bochev, Formulation, analysis and computation of an optimization-based local-to-nonlocal coupling method, *submitted*, 2018

WHAT ABOUT COUPLING?

Goal: merge two fundamentally different mathematical descriptions of the same physical phenomena: PDEs and nonlocal models



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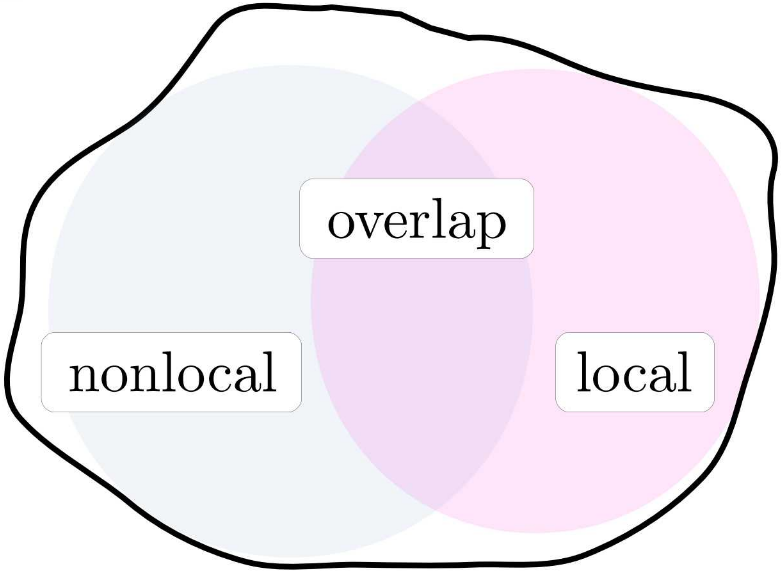

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Literature

(2012) Han and Lubineau: extension of the Arlequin method to continuum mechanics, **energy blending**

(2012) Lubineau et al.: morphing approach, **blending of material properties**

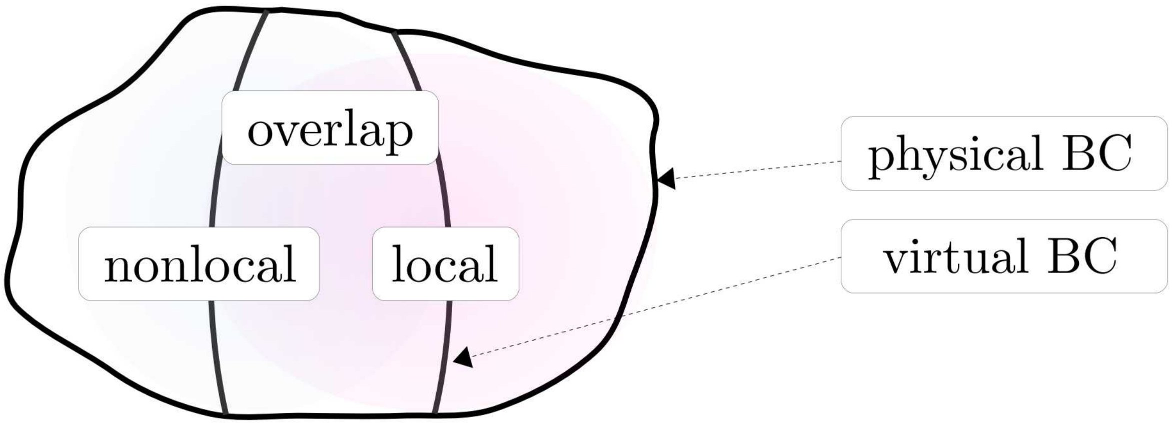
(2013) Seleson et al.: **force blending**

(2015) Silling et al.: **variable horizon**

(2017) Tian and Du.: heterogeneous localization via **nonlocal trace theorems**

WHAT ABOUT COUPLING?

Our strategy split the computational domain in a local and a nonlocal domain and **couple** the models at the interfaces or overlapping regions



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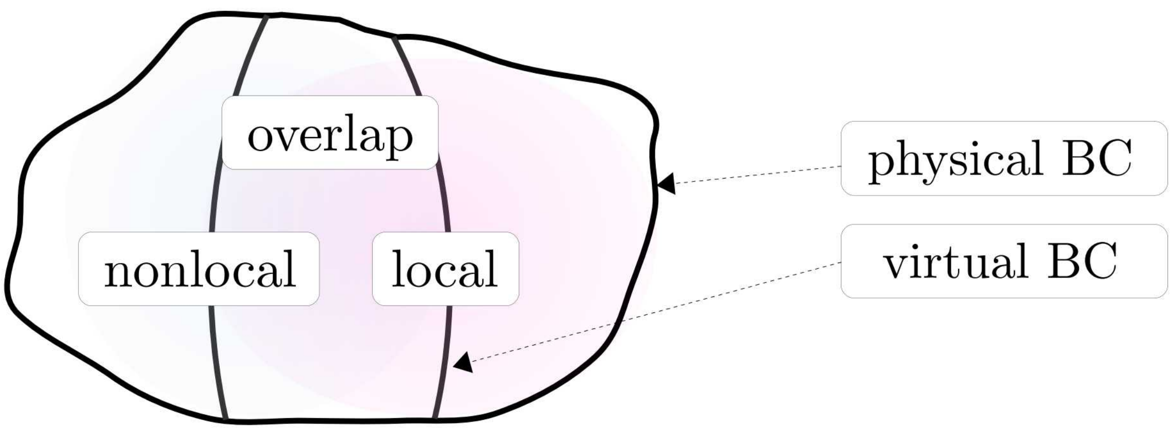


Contribution: design a coupling method that

- passes the patch test
- allows for separate softwares/solvers/meshes for the local and nonlocal problems

OUTLINE

- Notation
- The **Dirichlet** diffusion problem: formulation and analysis
- The **static peridynamic** problem
  1. formulation and finite dimensional approximation
  2. efficiency improvement
  3. from local to nonlocal boundary conditions

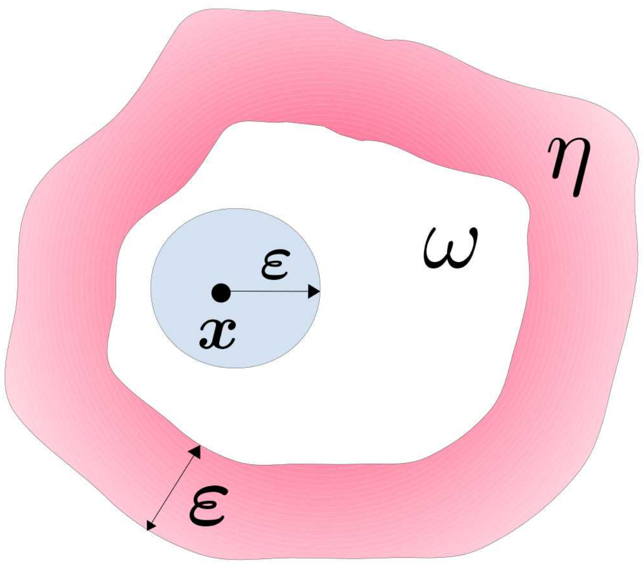
NOTATION

NONLOCAL VECTOR CALCULUS

Interaction domain of an open bounded region $\omega \in \mathbb{R}^d$

$$\eta = \{\boldsymbol{y} \in \mathbb{R}^d \setminus \omega : \; \boldsymbol{\alpha}(\boldsymbol{x},\boldsymbol{y}) \neq 0, \; \boldsymbol{x} \in \omega\},$$

Define: $\Omega = \omega \cup \eta$



Kernel: we assume

$$\begin{cases} \gamma(\boldsymbol{x},\boldsymbol{y}) \geq 0 & \forall\, \boldsymbol{y} \in B_\varepsilon(\boldsymbol{x}) \\ \gamma(\boldsymbol{x},\boldsymbol{y}) = 0 & \forall\, \boldsymbol{y} \in \Omega \setminus B_\varepsilon(\boldsymbol{x}), \end{cases}$$

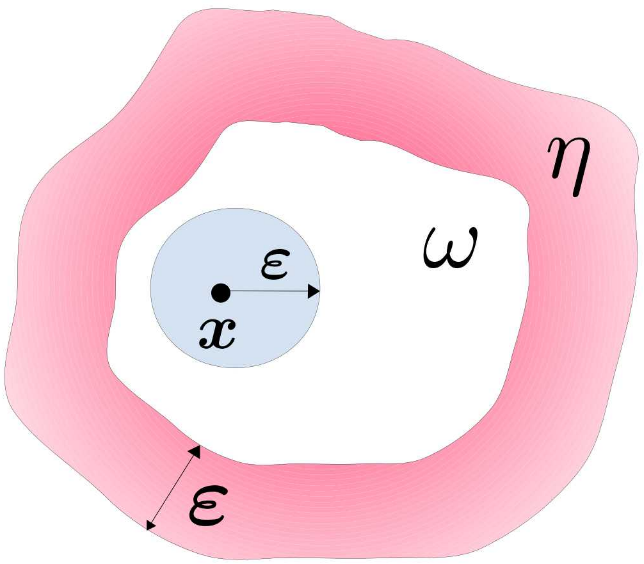
$$B_\varepsilon(\boldsymbol{x}) = \{\boldsymbol{y} \in \Omega : \; |\boldsymbol{x} - \boldsymbol{y}| \leq \varepsilon, \; \boldsymbol{x} \in \omega\}$$

PERIDYNAMICS/NONLOCAL ELASTICITY

kernel:

$$\gamma(\boldsymbol{x},\boldsymbol{y}) = C\,\frac{1}{|\boldsymbol{x}-\boldsymbol{y}|} \quad \text{for} \;\; |\boldsymbol{x}-\boldsymbol{y}| \le \varepsilon$$

$$\mathcal{L}u(\boldsymbol{x}) = C \int \frac{u(\boldsymbol{y}) - u(\boldsymbol{x})}{|\boldsymbol{x}-\boldsymbol{y}|}\, d\boldsymbol{y}$$



FRACTIONAL KERNELS

kernel:

$$\gamma(\boldsymbol{x},\boldsymbol{y}) = C\,\frac{1}{|\boldsymbol{x}-\boldsymbol{y}|^{n+2s}}, \quad s \in (0,1),\ \varepsilon = \infty$$

$$\mathcal{L}u(\boldsymbol{x}) = C\int \frac{u(\boldsymbol{y})-u(\boldsymbol{x})}{|\boldsymbol{x}-\boldsymbol{y}|^{n+2s}}\,d\boldsymbol{y}$$

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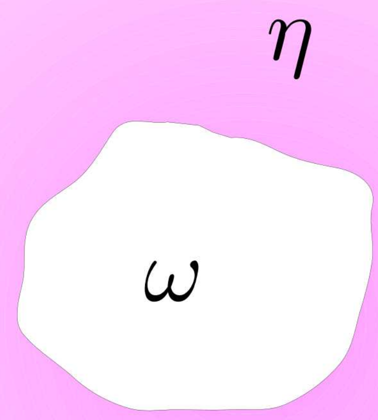
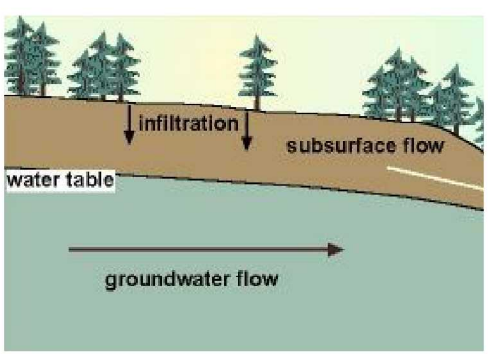


applications:

– stochastic jump processes (α stable Lévy processes

– subsurface flow, $s\in(0,1)$ is the **rate** of the
mean square displacement of the diffusing quantity



THE OPTIMIZATION PROBLEM

– M. D'Elia, M. Perego, P. Bochev, D. Littlewood, A coupling strategy for local and nonlocal diffusion models with mixed volume constraints and boundary conditions, *Computers and Mathematics with applications*, 2015

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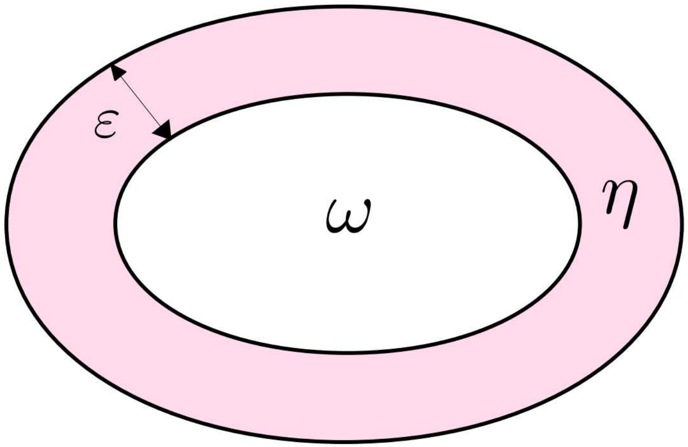
MODEL PROBLEMS

The nonlocal problem

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

where $\sigma_n \in \widetilde{V}(\eta)$ and $f_n \in L^2(\omega)$



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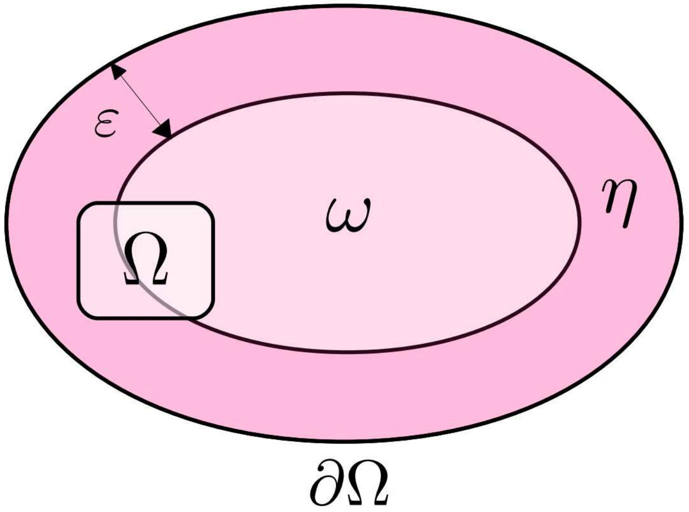

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where $\sigma_n \in \widetilde{V}(\eta)$ and $f_n \in L^2(\omega)$

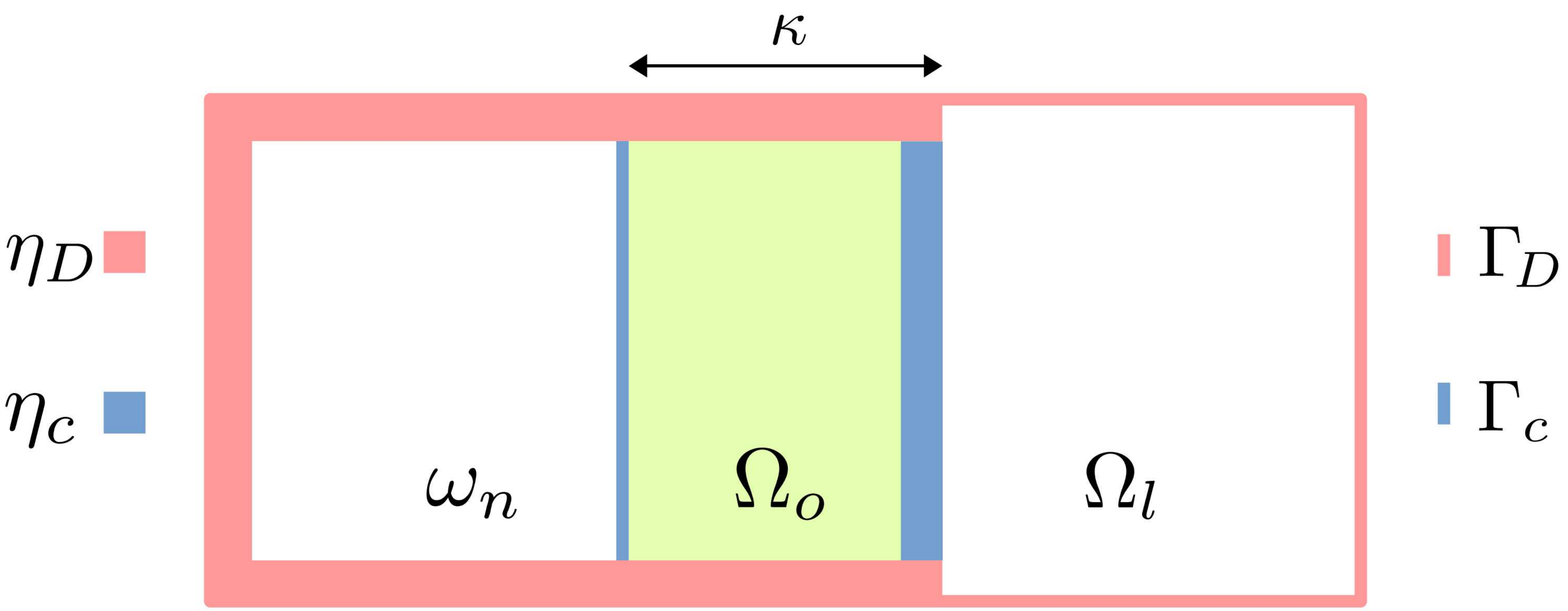
$\varepsilon \to 0$

The local problem: 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 $f_l \in L^2(\Omega)$

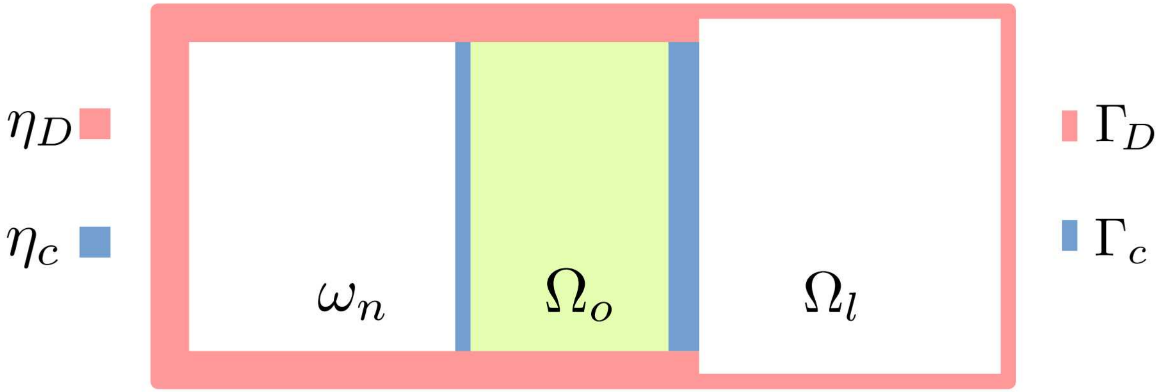
LtN COUPLING



LtN COUPLING

State equations

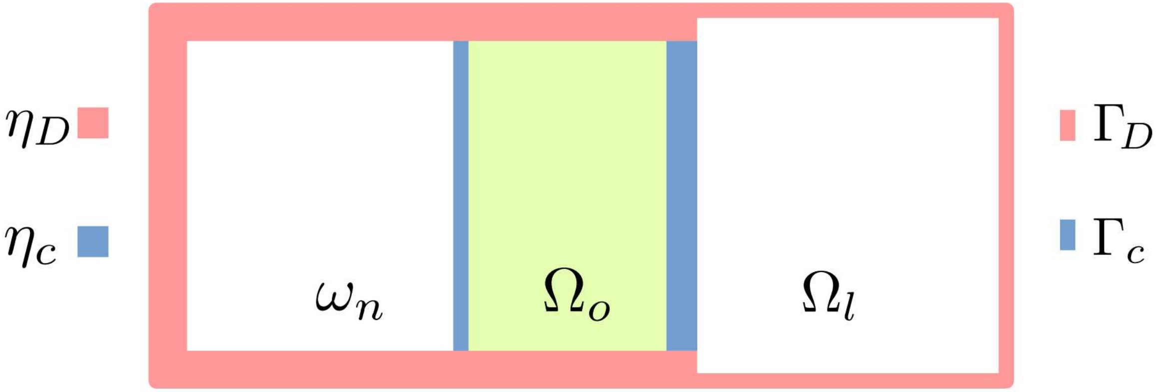
$$\begin{cases} -\mathcal{L}u_n = f_n & \boldsymbol{x} \in \omega_n \\ u_n = \theta_n & \boldsymbol{x} \in \eta_c \\ u_n = 0 & \boldsymbol{x} \in \eta_D \end{cases} \qquad \begin{cases} -\Delta u_l = f_l & \boldsymbol{x} \in \Omega_l \\ u_l = \theta_l & \boldsymbol{x} \in \Gamma_c \\ u_l = 0 & \boldsymbol{x} \in \Gamma_D \end{cases}$$



Optimization problem

$$\min_{u_n,u_l,\theta_n,\theta_l} J(u_n,u_l) = \min_{u_n,u_l,\theta_n,\theta_l} \frac{1}{2}\|u_n - u_l\|^2_{0,\Omega_o}$$

$$\text{s.t.} \left\{ \begin{array}{rcll} -\mathcal{L}u_n & = & f_n & \boldsymbol{x} \in \omega_n \\ u_n & = & \theta_n & \boldsymbol{x} \in \eta_c \\ u_n & = & 0 & \boldsymbol{x} \in \eta_D \end{array} \right. \qquad \left\{ \begin{array}{rcll} -\Delta u_l & = & f_l & \boldsymbol{x} \in \Omega_l \\ u_l & = & \theta_l & \boldsymbol{x} \in \Gamma_c \\ u_l & = & 0 & \boldsymbol{x} \in \Gamma_D \end{array} \right.$$



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LtN COUPLING

LtN solution

- optimal solution: $(\theta_n^*, \theta_l^*) \in \Theta_n \times \Theta_l$
- LtN solution: $= \begin{cases} u_n^*(\theta_n^*) & \boldsymbol{x} \in \Omega_n \\ u_l^*(\theta_l^*) & \boldsymbol{x} \in \Omega_l \setminus \Omega_o \end{cases}$

IS THE SOLUTION UNIQUE?

Reduced form:

$$\min_{\theta_n,\theta_l} J(\theta_n,\theta_l) = \min_{\theta_n,\theta_l} \frac{1}{2}\|u_n(\theta_n) - u_l(\theta_l)\|^2_{0,\Omega_o}$$

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Solution splitting:

$$u_n = v_n(\theta_n) + u_n^0 \qquad \text{and} \qquad u_l = v_l(\theta_l) + u_l^0$$

harmonic components v_n and v_l

$$\begin{cases} -\mathcal{L}v_n & = 0 & \boldsymbol{x} \in \omega_n \\ \quad v_n & = \theta_n & \boldsymbol{x} \in \eta_c \\ +\mathrm{VC} \end{cases} \quad \text{and} \quad \begin{cases} -\Delta v_l & = 0 & \boldsymbol{x} \in \Omega_l \\ \quad v_l & = \theta_l & \boldsymbol{x} \in \Gamma_c \\ +\mathrm{BC} \end{cases}$$

homogeneous components u_n^0 and u_l^0

$$\begin{cases} -\mathcal{L}u_n^0 & = f_n & \boldsymbol{x} \in \omega_n \\ \quad v_n & = 0 & \boldsymbol{x} \in \eta_c \\ +\mathrm{VC} \end{cases} \quad \text{and} \quad \begin{cases} -\Delta u_l^0 & = f_l & \boldsymbol{x} \in \Omega_l \\ \quad v_l & = 0 & \boldsymbol{x} \in \Gamma_l \\ +\mathrm{BC} \end{cases}$$

IS THE SOLUTION UNIQUE?

Reduced functional:

$$J(\theta_n, \theta_l) = \frac{1}{2}\|v_n(\theta_n) - v_l(\theta_l)\|^2_{0,\Omega_o} + \big(u_n^0 - u_l^0, v_n(\theta_n) - v_l(\theta_l)\big)_{0,\Omega_o}$$

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Lemma: The reduced space problem has a **unique** solution

IS THE SOLUTION UNIQUE?

Reduced functional:

$$J(\theta_n,\theta_l) = \frac{1}{2}\underbrace{\|v_n(\theta_n)-v_l(\theta_l)\|^2_{0,\Omega_o}}_{Q(\theta_n,\theta_l;\theta_n,\theta_l) = \|(\theta_n,\theta_l)\|_*} + \left(u_n^0-u_l^0, v_n(\theta_n)-v_l(\theta_l)\right)_{0,\Omega_o}$$

Lemma: The reduced space problem has a **unique** solution

Key result: $\displaystyle\int_{\Omega_o} \left(v_n(\sigma_n) - v_l(\sigma_l)\right)\left(v_n(\mu_n) - v_l(\mu_l)\right) := ((\sigma_n,\sigma_l),(\mu_n,\mu_l))_*$

defines an **inner product** in the control variable space

$$\Rightarrow \|v_n(\theta_n)-v_l(\theta_l)\|^2_{0,\Omega_o} := \|(\sigma_n,\sigma_l)\|_*$$

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Careful: The control space is not necessarily complete $\Rightarrow$ consider a **completion**

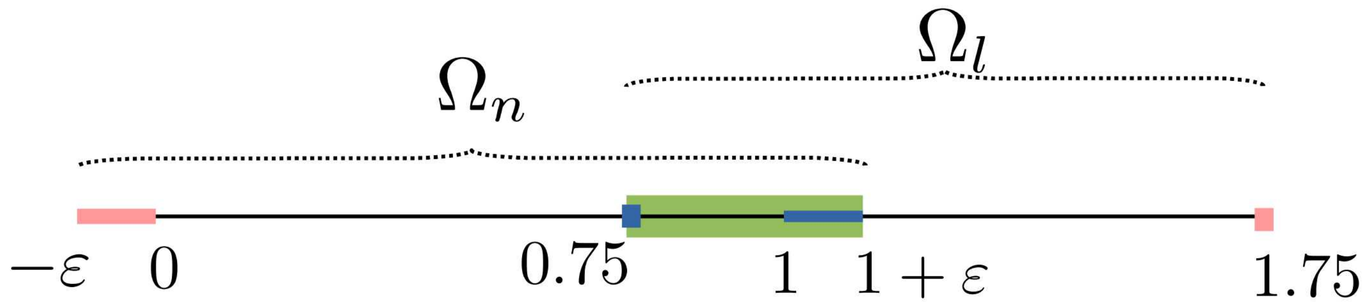
FINITE DIMENSIONAL APPROXIMATION

discretization: 1D finite element method (piece-wise continuous and discontinuous)

analysis: convergence rates are the same obtained by discretization of the states

results:

- polynomial patch tests
- accuracy results
- valid for several kernel choices



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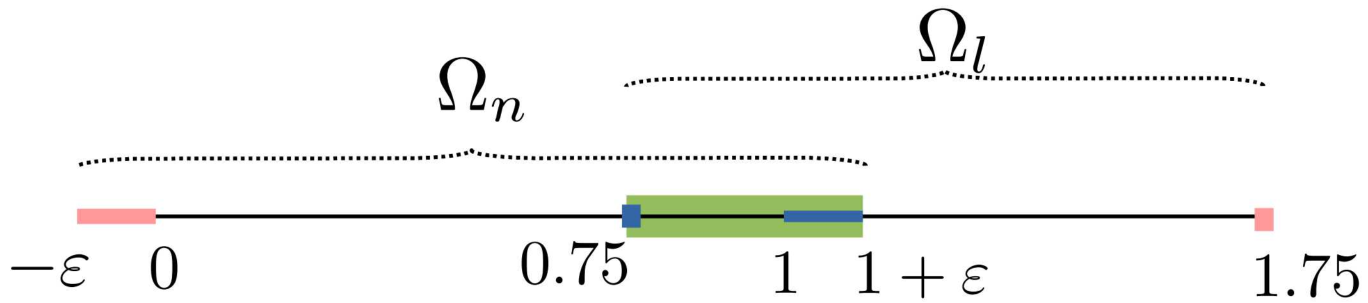
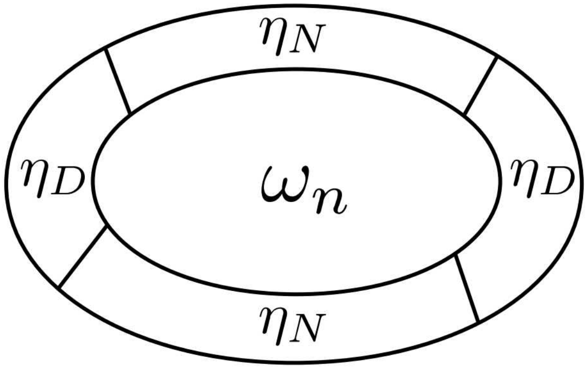


STATIC NONLOCAL ELASTICITY

– M. D'Elia, P. Bochev, D. Littlewood, M. Perego, Optimization-based coupling of local and nonlocal models: Applications to peridynamics, *Chapter in Handbook of nonlocal continuum mechanics for materials and structures, Springer*, 2017

THE PERIDYNAMIC MODEL

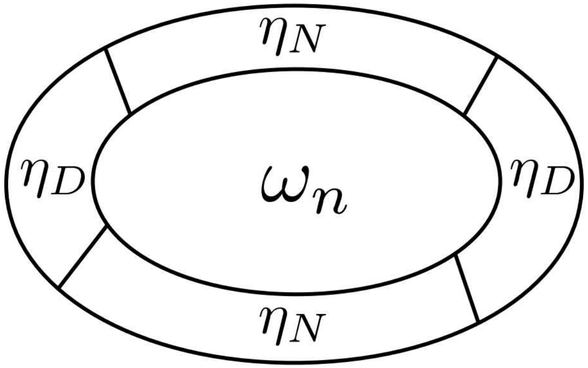


Peridynamic (PD) equilibrium equation:

$$-\mathcal{L}[\mathbf{u}](\boldsymbol{x}) := -\int_{\Omega} \{\mathbf{T}[\boldsymbol{x}]\langle \boldsymbol{x}' - \boldsymbol{x}\rangle - \mathbf{T}[\boldsymbol{x}']\langle \boldsymbol{x} - \boldsymbol{x}'\rangle\}\, dV_{\boldsymbol{x}'} = \mathbf{b}(\boldsymbol{x})$$

$\mathbf{u}$: displacement field, $\mathbf{b}$: given body force, $\mathbf{T}$: force state field

THE PERIDYNAMIC MODEL



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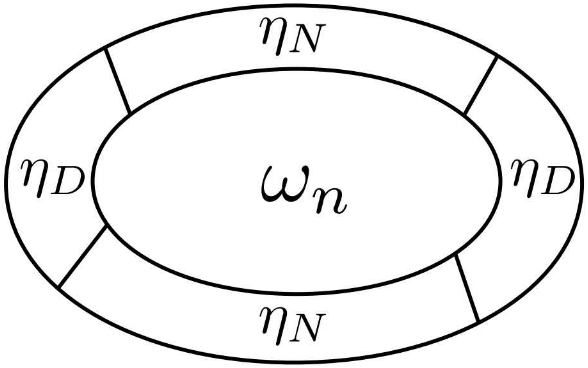
PD equation:
$$\begin{cases} -\mathcal{L}_{\mathrm{LPS}}[\mathbf{u}](\boldsymbol{x}) = \mathbf{b}(\boldsymbol{x}) & \boldsymbol{x} \in \omega_n, \\ \mathbf{u}(\boldsymbol{x}) = \mathbf{g}(\boldsymbol{x}) & \boldsymbol{x} \in \eta_D, \\ -\mathcal{N}(\mathbf{u}(\boldsymbol{x})) = \eta_n & \boldsymbol{x} \in \eta_N \end{cases}$$

THE PERIDYNAMIC MODEL



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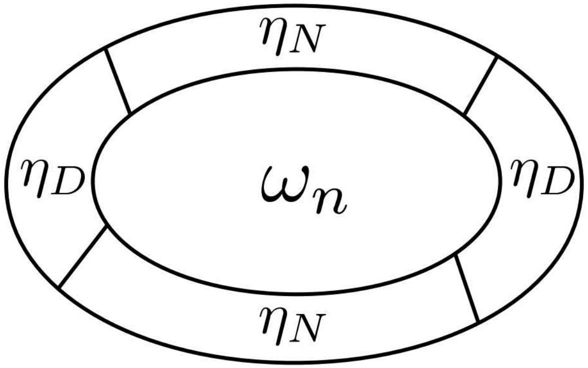
Local equation: $-\mathcal{L}_{\mathrm{NC}}[\mathbf{u}](\boldsymbol{x}) = \mathbf{b}(\boldsymbol{x})$, where $\mathcal{L}_{\mathrm{NC}}$ is Navier-Cauchy model

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

THE PERIDYNAMIC MODEL



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PD equation:

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

- equivalent for quadratic fields
- for $\varepsilon \to 0$, **PD** $\to$ **NC**

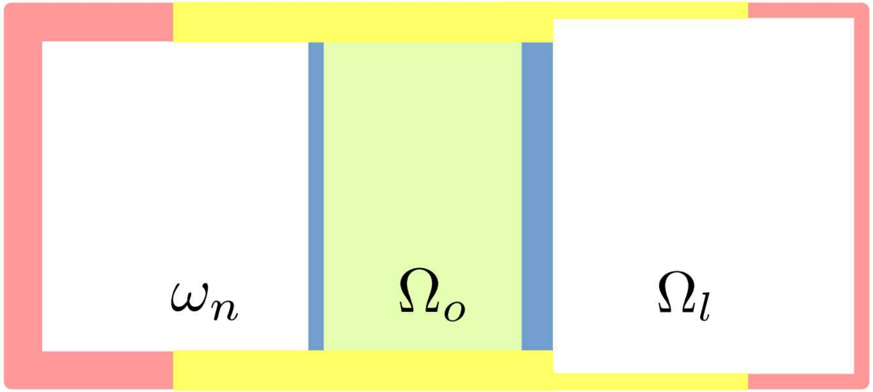
Local equation: $-\mathcal{L}_{\mathrm{NC}}[\mathbf{u}](\boldsymbol{x}) = \mathbf{b}(\boldsymbol{x})$, where $\mathcal{L}_{\mathrm{NC}}$ is Navier-Cauchy model

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

Optimization-based coupling

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

$$\text{s.t.} \left\{ \begin{aligned} -\mathcal{L}_{\rm LPS}[\mathbf{u}_n] &= \mathbf{b} & \boldsymbol{x} &\in \omega_n \\ \mathbf{u}_n &= \mathbf{0} & \boldsymbol{x} &\in \eta_D \\ -\mathcal{N}(\mathbf{u}_n) &= 0 & \boldsymbol{x} &\in \eta_N \\ \mathbf{u}_n &= \boldsymbol{\nu}_n & \boldsymbol{x} &\in \eta_c \end{aligned} \right. \qquad \left\{ \begin{aligned} -\mathcal{L}_{\rm NC}[\mathbf{u}_l] &= \mathbf{b} & \boldsymbol{x} &\in \Omega_l \\ \mathbf{u}_l &= \mathbf{0} & \boldsymbol{x} &\in \Gamma_D \\ -\nabla\mathbf{u}_l \cdot \mathbf{n} &= 0 & \boldsymbol{x} &\in \Gamma_N \\ \mathbf{u}_l &= \boldsymbol{\nu}_l & \boldsymbol{x} &\in \Gamma_c \end{aligned} \right.$$



THE COUPLING STRATEGY

Optimization-based coupling

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

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Discretization:

local problem: variational form with FEM

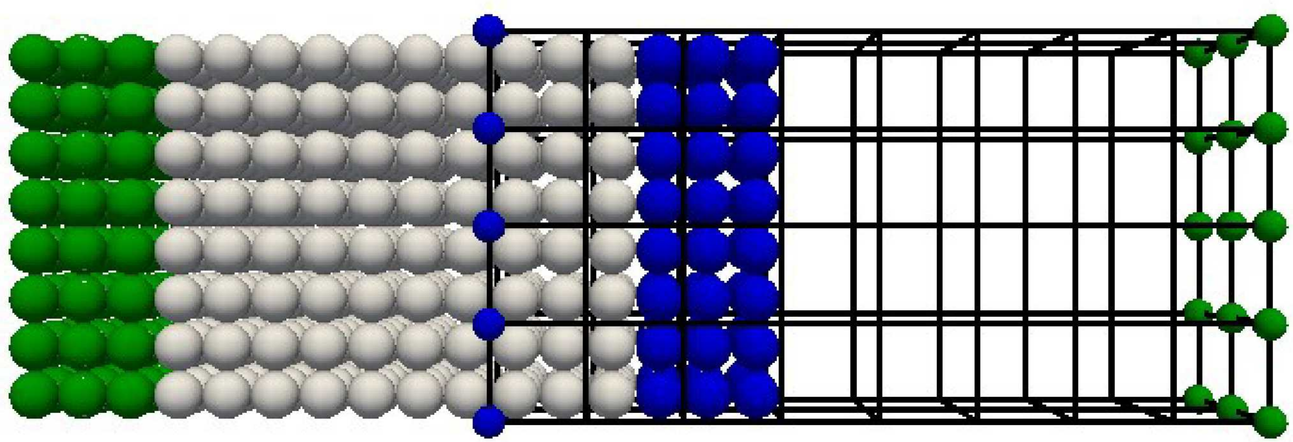
nonlocal problem: strong form with mesh free method

$$L[\boldsymbol{x}_i] := \sum_{j\in\mathcal{N}_i} \{\mathbf{T}[\boldsymbol{x}_i]\langle\boldsymbol{x}_j-\boldsymbol{x}_i\rangle - \mathbf{T}[\boldsymbol{x}_j]\langle\boldsymbol{x}_i-\boldsymbol{x}_j\rangle\}\, V_j^{(i)}, \qquad V_j^{(i)} = |B_\varepsilon(\boldsymbol{x}_i)\cap B_\varepsilon(\boldsymbol{x}_j)|$$

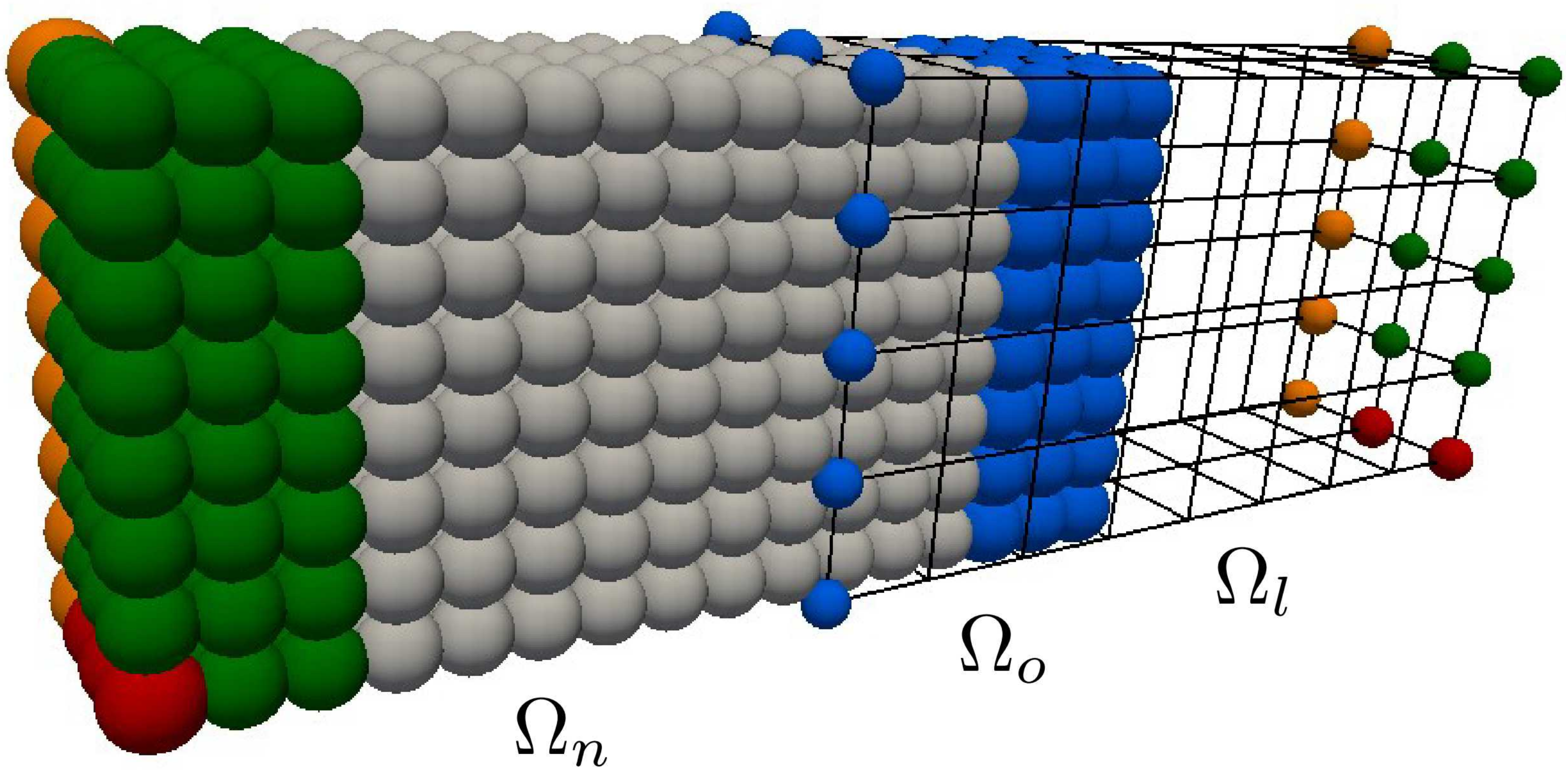
GEOMETRY

Coupling Peridigm and Albany

peridigm.sandia.gov   software.sandia.gov/albany/   trilinos.org/packages/rol



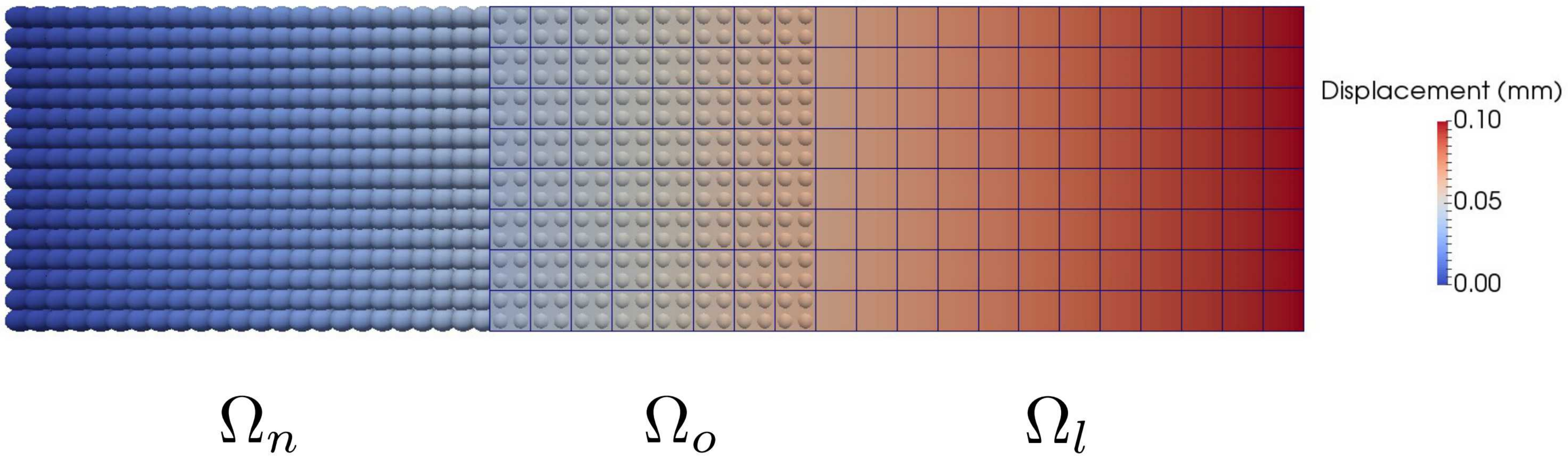
THE GEOMETRY



THE PATCH TEST

Analytic solution: $\mathbf{u} = 10^{-3}(x, 0, 0)$, **linear** patch test, $\mathbf{b}(\mathbf{x}) = \mathbf{0}$

$$\Omega = [0,\ 100] \times [-12.5,\ 12.5] \times [-12.5,\ 12.5]\ \text{mm}^3$$



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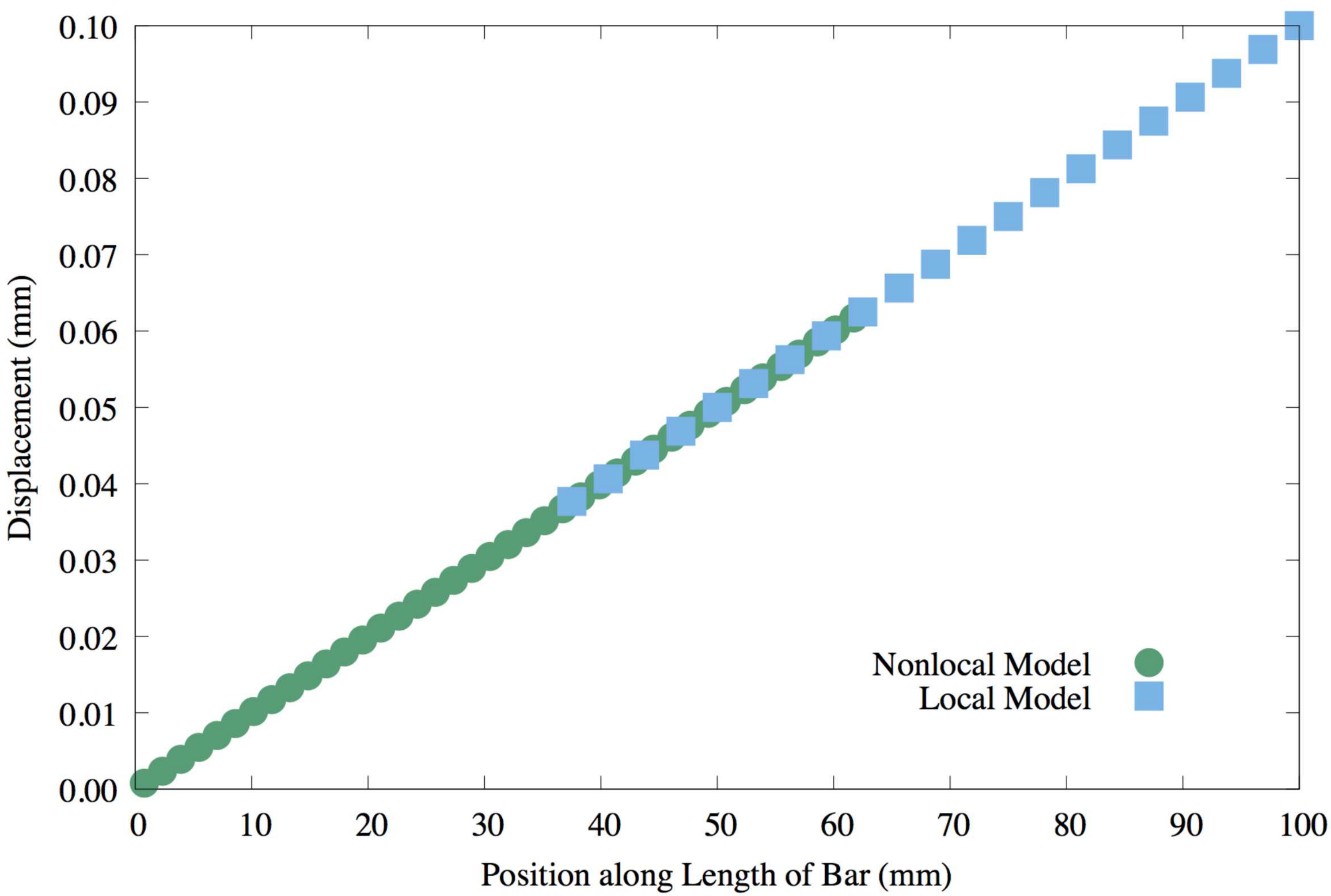


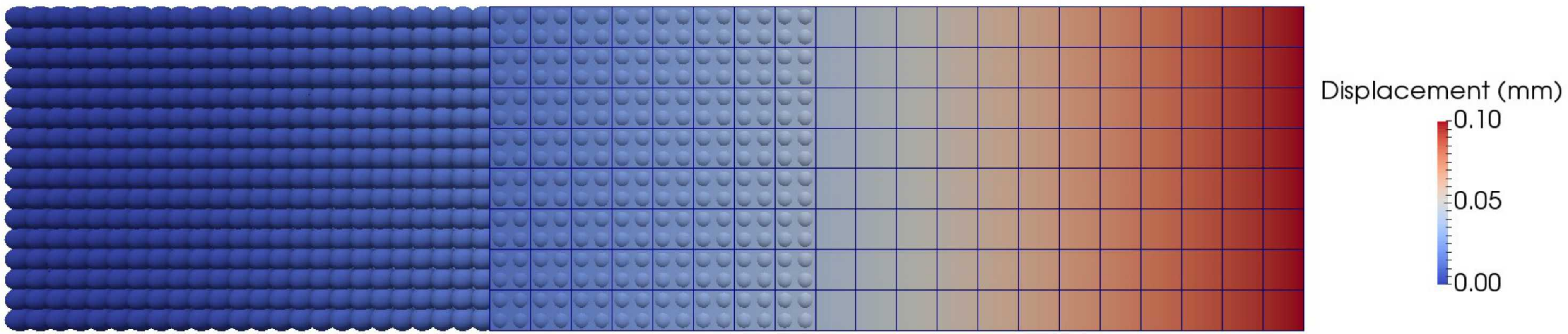
THE PATCH TEST

Analytic solution: $\mathbf{u} = 10^{-5}(x^2, 0, 0)$, **quadratic** patch test

$K = 150\text{GPa}$, $G = 81.496\text{GPa}$ (stainless steel), $\varepsilon = 4.270\text{mm}$

$\mathbf{b} = 10^{-5}(\frac{8G}{3} + 2K) = 5.173\,\text{N}\text{mm}^{-3}$

$\Omega = [0,\ 100] \times [-12.5,\ 12.5] \times [-12.5,\ 12.5]\,\text{mm}^3$



Ω_n Ω_o Ω_l

THE PATCH TEST

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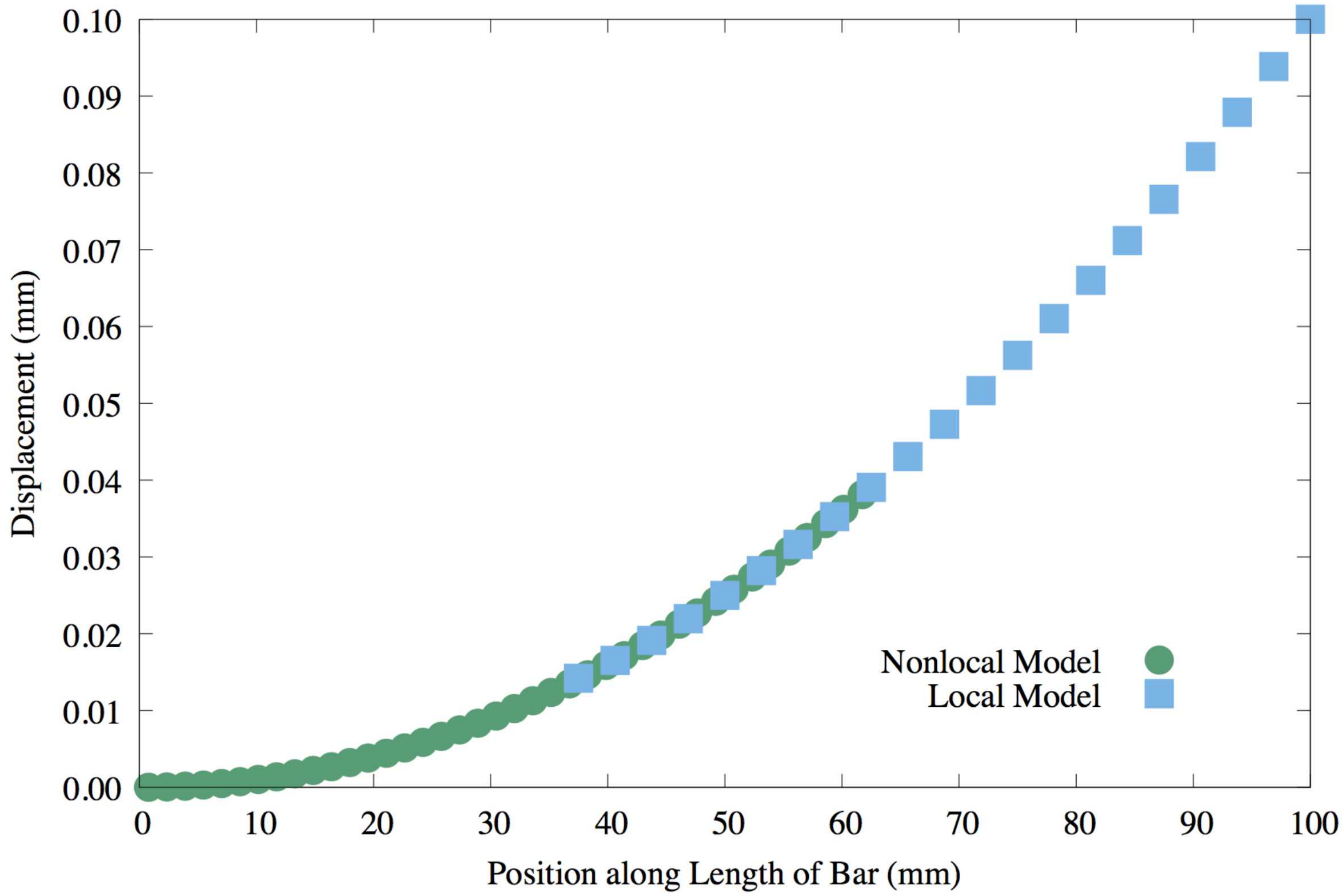
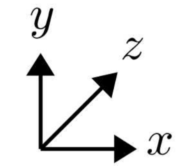
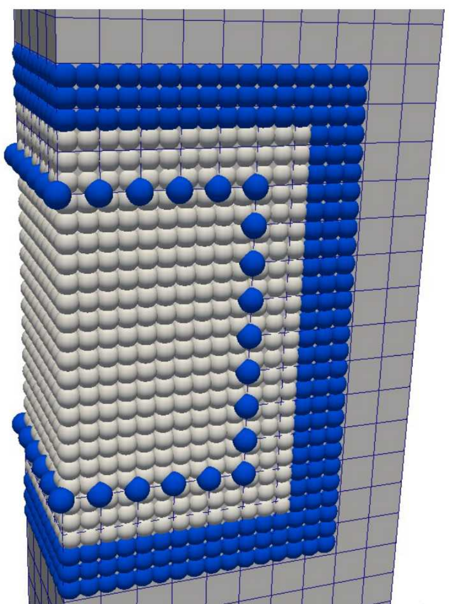


TENSILE BAR

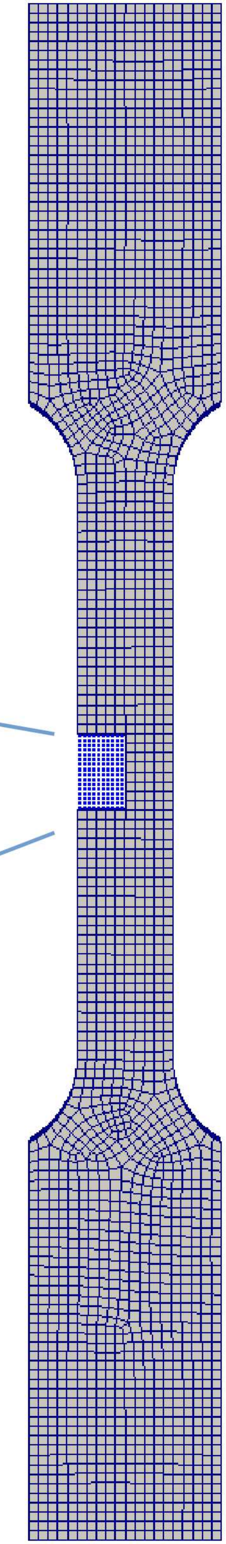


Dimensions: height=100mm, width at mid point=6.25mm

Parameters: $K = 160\text{GPa}$, $G = 81.496\text{GPa}$, $\varepsilon = 0.54\text{mm}$



control nodes



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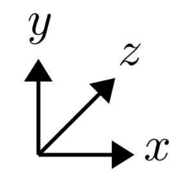

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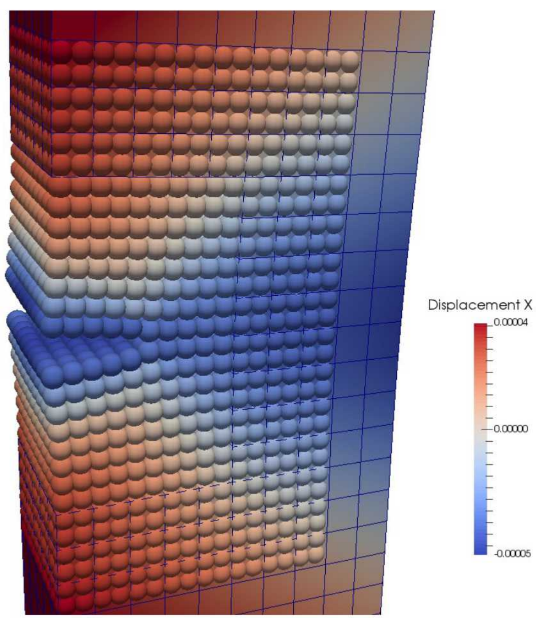

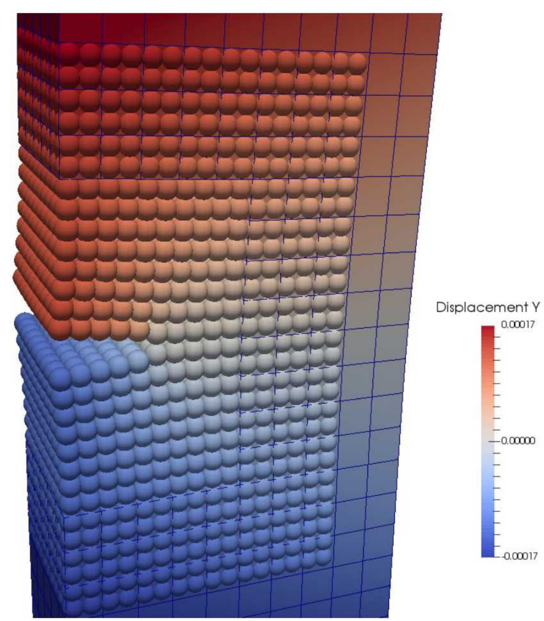

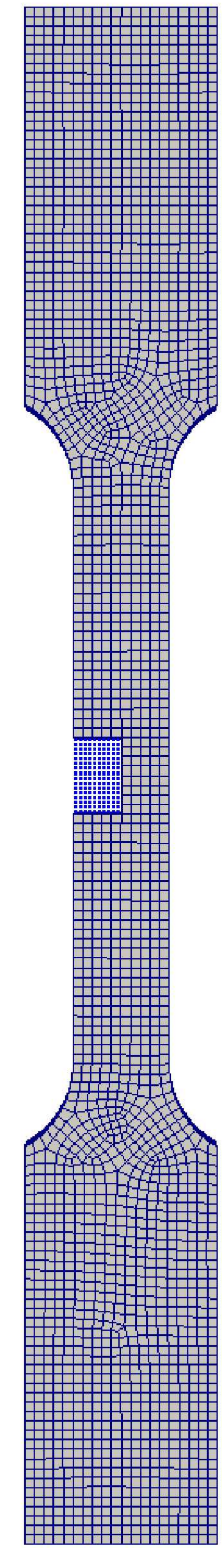

ANOTHER CRACK TEST

Boundary conditions: Neumann on the left, Dirichlet on the right along the x direction.

how can we guess nonlocal Neumann conditions???

pressure conditions can only be obtained on a surface

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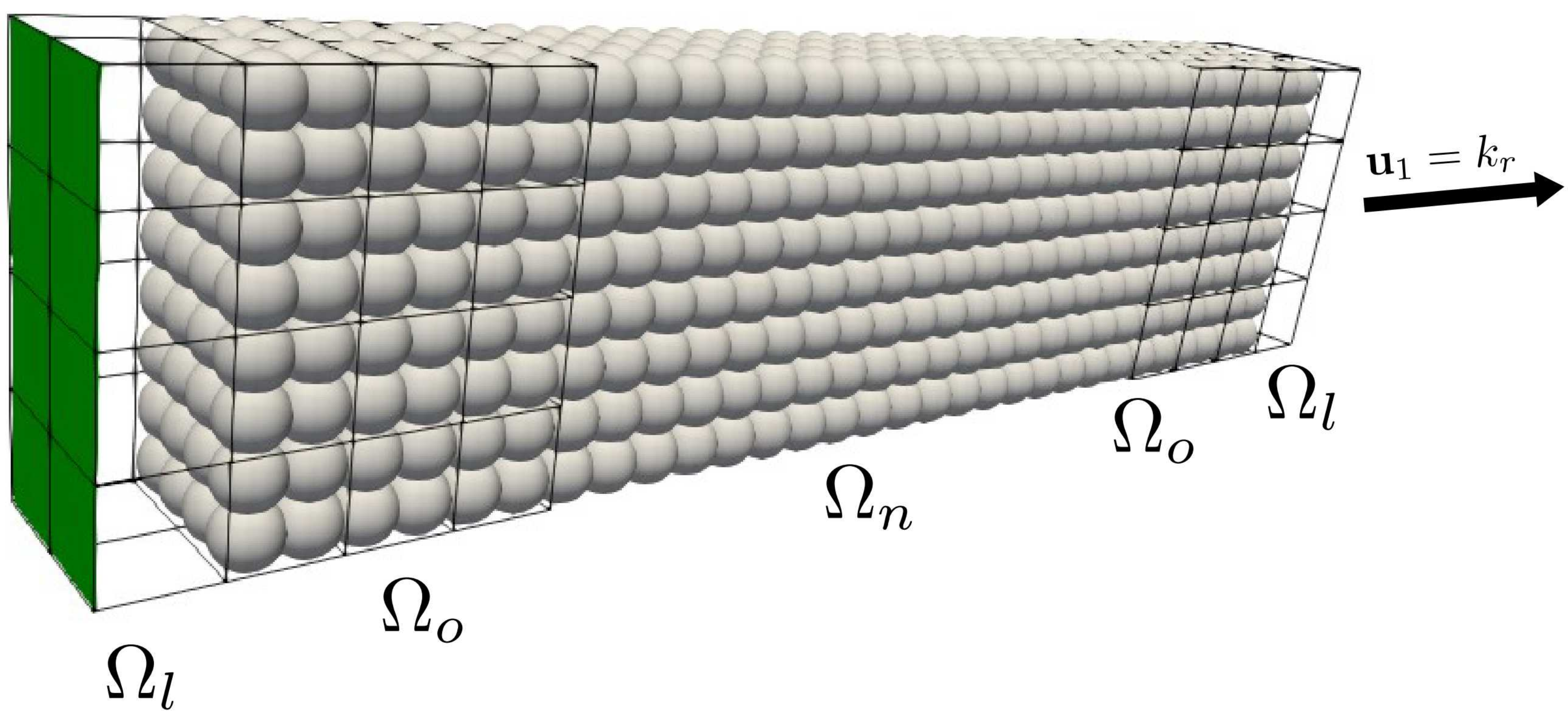
Neumann:
$p = -\overline{p}$



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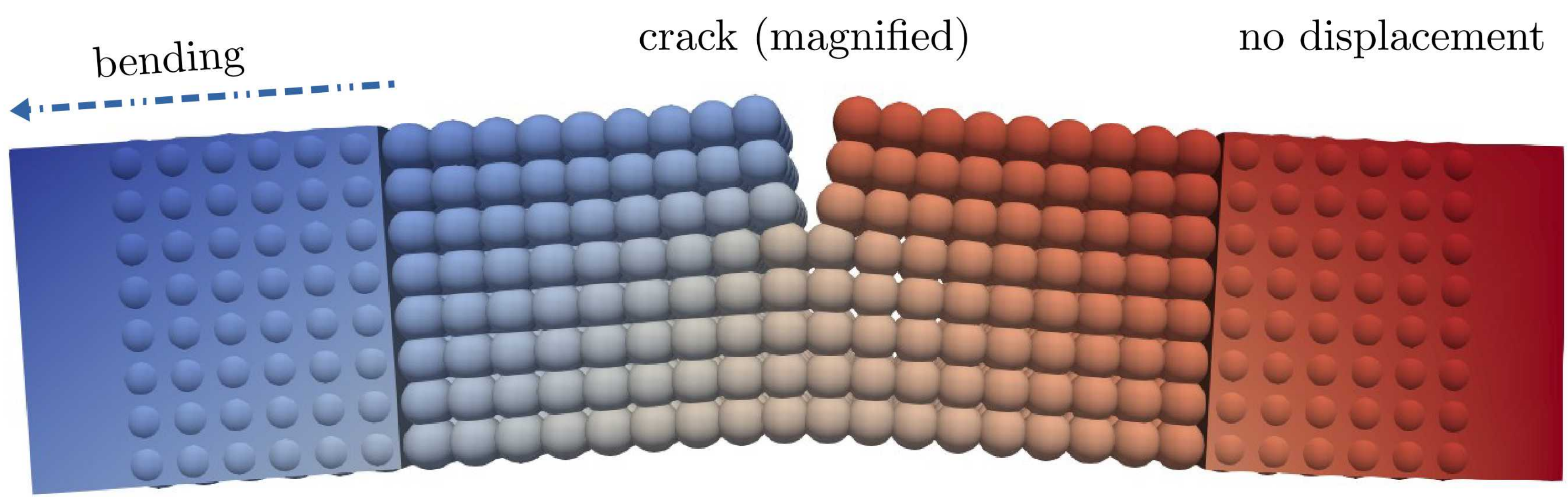
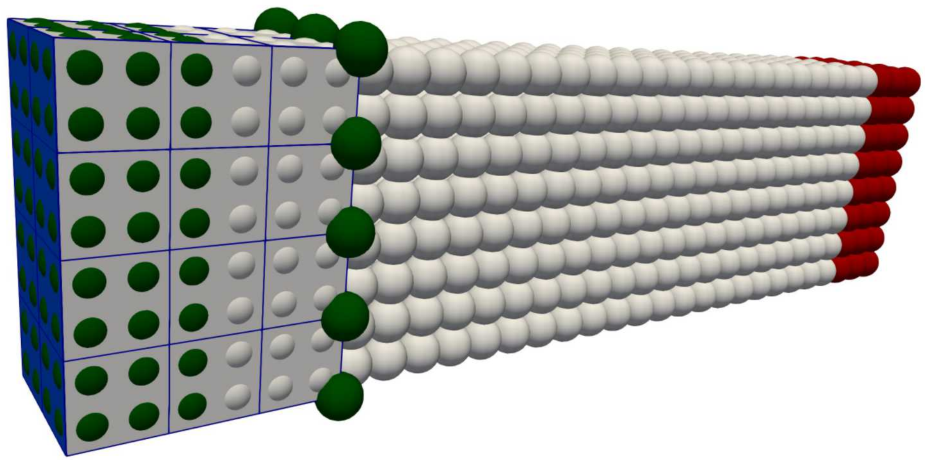


DEALING WITH LOCAL BC

geometry: the overlap and local domains coincide

local **Neumann** boundary condition

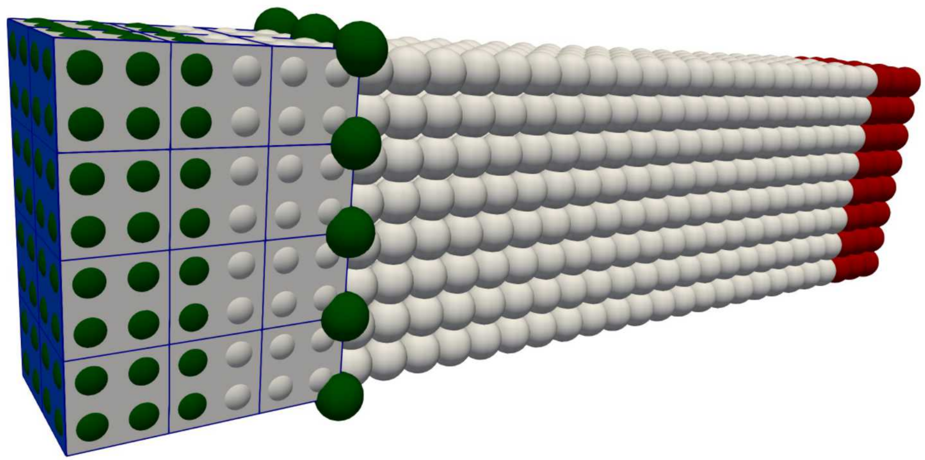


Dirichlet nodes

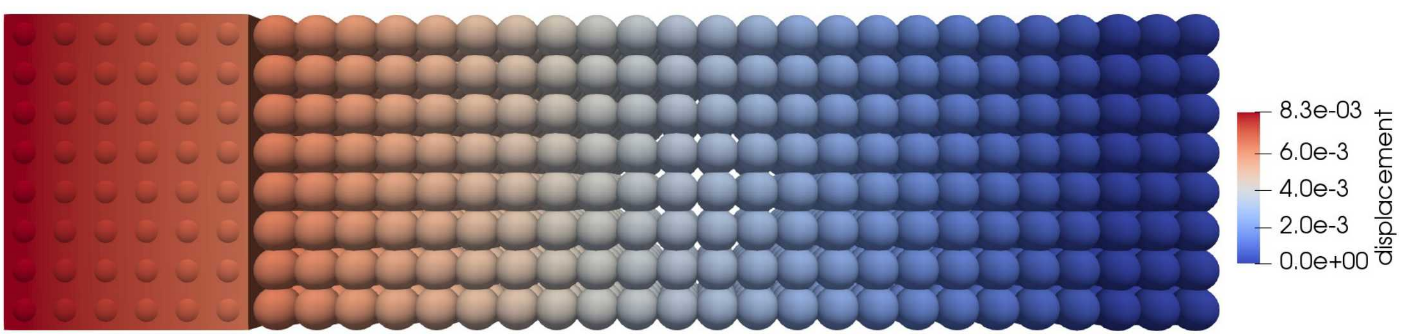
overlap

DEALING WITH LOCAL BC

geometry: the overlap and local domains coincide



coupled solution: linear elongation

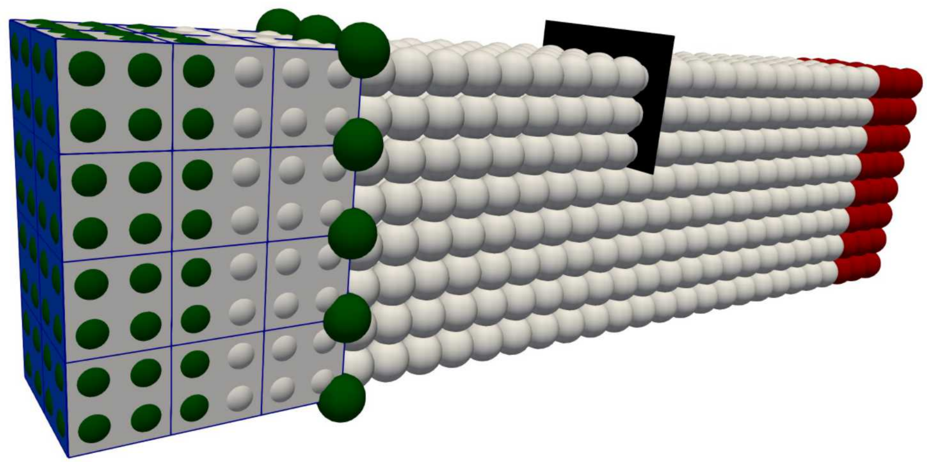


Displacements magnified 5x for visualization purposes

DEALING WITH LOCAL BC

geometry with crack: the overlap and local domains coincide

local
Neumann
boundary
condition



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DEALING WITH LOCAL BC

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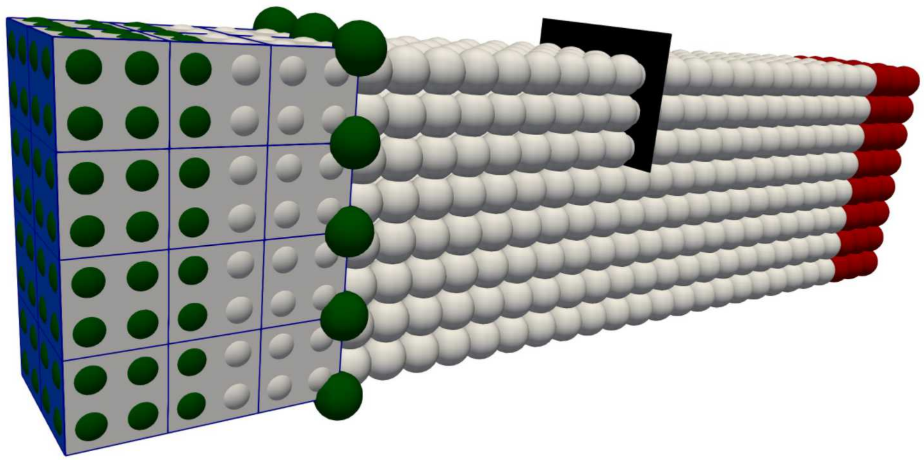

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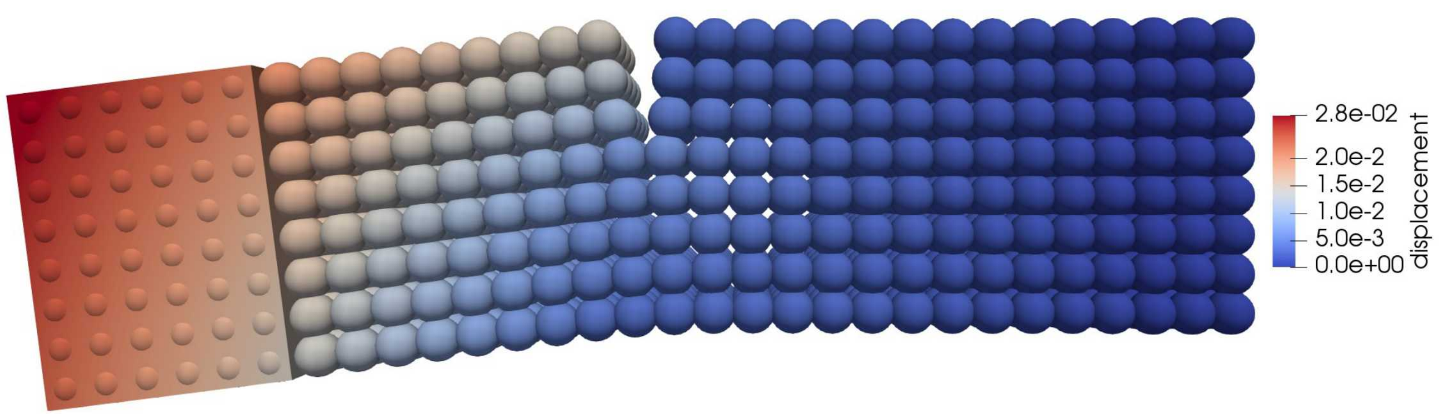
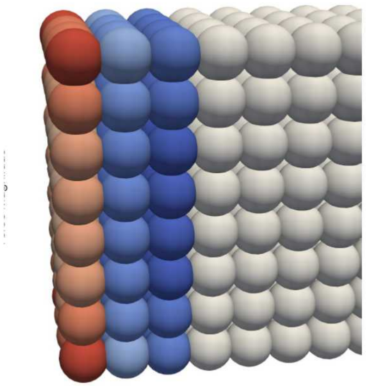
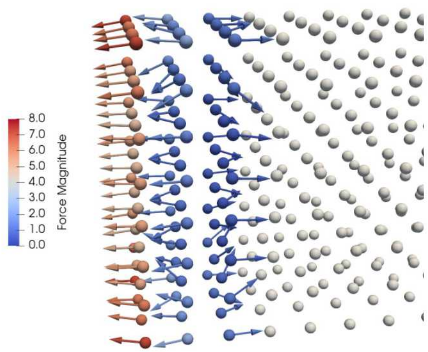


DEALING WITH LOCAL BC

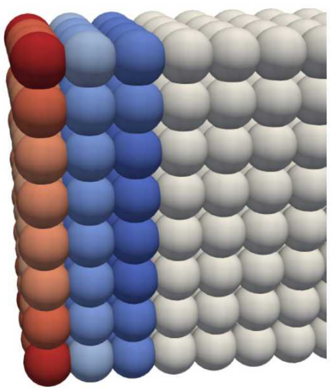
NO crack

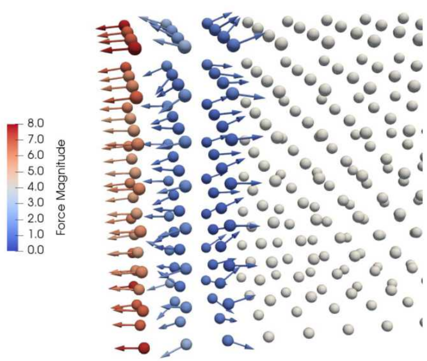




what: unbalanced forces on control nodes in the nonlocal domain **(post processing)**

WITH crack





DEALING WITH LOCAL BC

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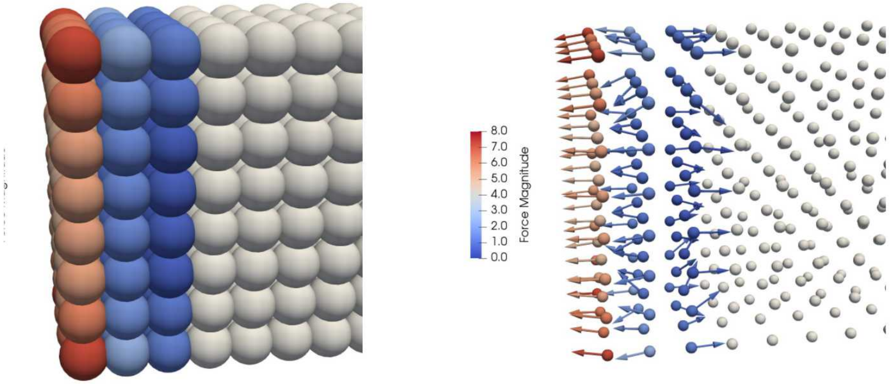
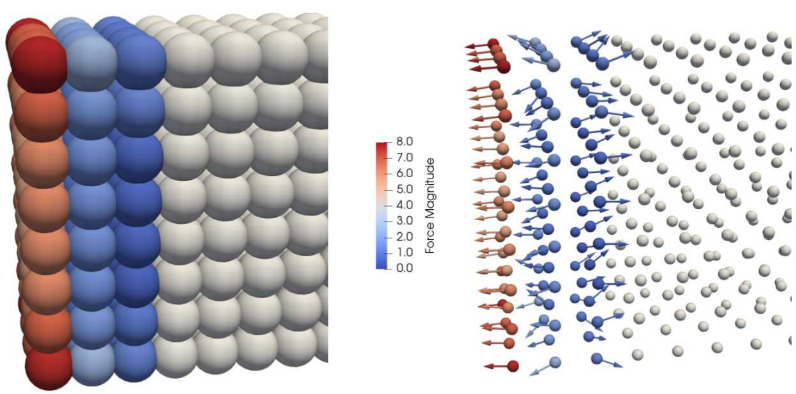


what: unbalanced forces on control nodes in the nonlocal domain **(post processing)**

accomplishment: converted a local traction on a surface to nonlocal body forces

(applied individually to each node in the volumetric boundary layer)

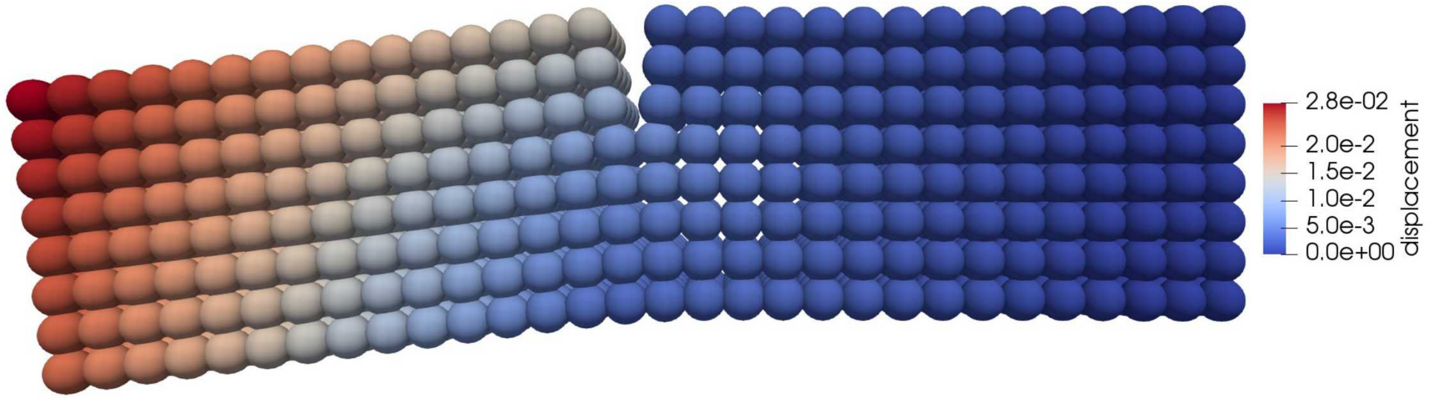
WITH crack



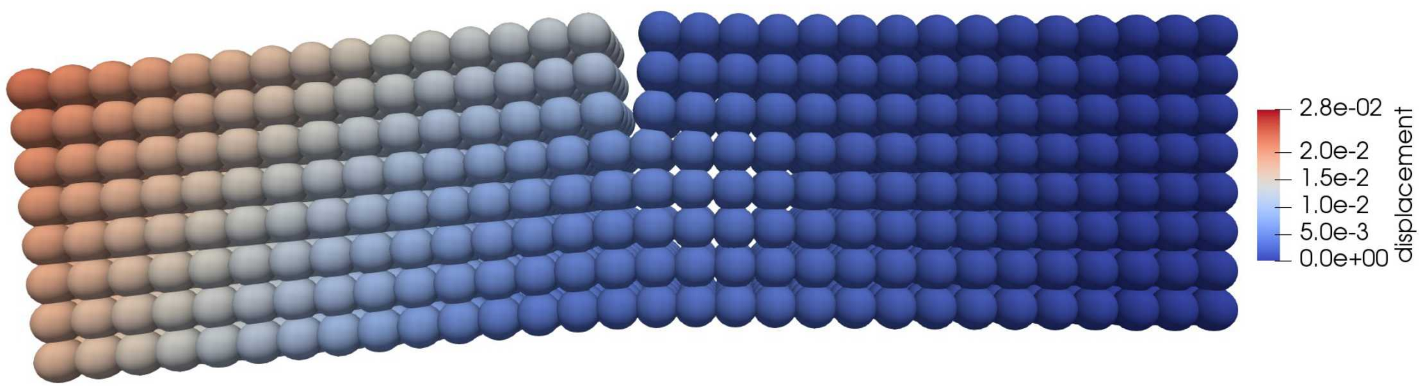
question: can we **reuse** these forces in similar simulations **without** coupling?

DEALING WITH LOCAL BC

coupled solution with Neumann data



purely nonlocal with forces obtained from coupled solution **without** crack



note: solutions are different but results are encouraging!

Thank you

THE PERIDYNAMIC MODEL

THE PERIDYNAMIC MODEL

Time-dependent problem:

$$\rho(\boldsymbol{x},t)\,\frac{\partial^2\mathbf{u}}{\partial t^2}(\boldsymbol{x},t) = \int_\Omega \left\{\mathbf{T}[\boldsymbol{x},t]\langle\boldsymbol{x}'-\boldsymbol{x}\rangle - \ \mathbf{T}[\boldsymbol{x}',t]\langle\boldsymbol{x}-\boldsymbol{x}'\rangle\right\} dV'_{\boldsymbol{x}} + \mathbf{b}(\boldsymbol{x},t)$$

$\rho\colon \Omega\times\mathbb{R}^+\to\mathbb{R}^+$: mass density
$\mathbf{u}\colon \Omega\times\mathbb{R}^+\to\mathbb{R}^3$: displacement field
$\mathbf{b}\colon \Omega\times\mathbb{R}^+\to\mathbb{R}^3$: given body force density
$\mathbf{T}\colon \Omega\times\mathbb{R}^+\to\mathbb{R}^{(3,3)}$: force state field $\longrightarrow$ force state at $(\boldsymbol{x},t)$ mapping the bond $\langle\boldsymbol{x}'-\boldsymbol{x}\rangle$ to force per unit volume squared

Static:

$$-\mathcal{L}[\mathbf{u}](\boldsymbol{x}) := -\int_\Omega \left\{\mathbf{T}[\boldsymbol{x}]\langle\boldsymbol{x}'-\boldsymbol{x}\rangle - \mathbf{T}[\boldsymbol{x}']\langle\boldsymbol{x}-\boldsymbol{x}'\rangle\right\} dV'_{\boldsymbol{x}} = \mathbf{b}(\boldsymbol{x})$$

THE PERIDYNAMIC MODEL

$$\mathbf{T}[\boldsymbol{x}]\langle \boldsymbol{x}' - \boldsymbol{x} \rangle = 0, \quad \forall\, \boldsymbol{x}' \notin B_\delta(\boldsymbol{x})$$

averaging bond elongation

$$\mathbf{T}[\boldsymbol{x}]\langle \boldsymbol{\xi} \rangle = \frac{w(|\boldsymbol{\xi}|)}{m} \left\{ (3K - 5G)\, \theta(\boldsymbol{x}) \boldsymbol{\xi} + 15G \frac{\boldsymbol{\xi} \otimes \boldsymbol{\xi}}{|\boldsymbol{\xi}|^2} (\mathbf{u}(\boldsymbol{x} + \boldsymbol{\xi}) - \mathbf{u}(\boldsymbol{x})) \right\} \qquad \forall\, \boldsymbol{x} \in \Omega,\ \boldsymbol{\xi} = \boldsymbol{x}' - \boldsymbol{x}$$

volume change, dilatation

deviation, shear

K: bulk modulus, G: shear modulus

$\theta : \Omega \to \mathbb{R}$, linearized nonlocal dilatation

$$\theta(\boldsymbol{x}) = \frac{3}{m} \int_{B_\delta(\mathbf{0})} w(|\boldsymbol{\zeta}|)\, \boldsymbol{\zeta} \cdot (\mathbf{u}(\boldsymbol{x} + \boldsymbol{\zeta}) - \mathbf{u}(\boldsymbol{x}))\, dV_{\boldsymbol{\zeta}}$$

$$m = \int_{B_\delta(\mathbf{0})} w(|\boldsymbol{\zeta}|)\, |\boldsymbol{\zeta}|^2\, dV_{\boldsymbol{\zeta}}$$

w: spherical influence function, scalar valued function that determines the support of force states and modulates the bond strength

1D FINITE DIMENSIONAL APPROXIMATION

– M. D'Elia, P. Bochev, Formulation, analysis and computation of an optimization-based local-to-nonlocal coupling method, *submitted*, 2018

THE ALGORITHM

Optimization problem

$$\min_{u_n, u_l, \theta_n, \theta_l} \quad \frac{1}{2}\|u_n - u_l\|^2_{0,\Omega_o}$$

$$\text{s.t.} \begin{cases} -\mathcal{L}u_n & = & f_n & \boldsymbol{x} \in \omega_n \\ u_n & = & \theta_n & \boldsymbol{x} \in \eta_c \\ u_n & = & 0 & \boldsymbol{x} \in \eta_D \end{cases} \qquad \begin{cases} -\Delta u_l & = & f_l & \boldsymbol{x} \in \Omega_l \\ u_l & = & \theta_l & \boldsymbol{x} \in \Gamma_c \\ u_l & = & 0 & \boldsymbol{x} \in \Gamma_D \end{cases}$$

weak form + FEM

$$\int_{\Omega_n}\int_{\Omega_n} \mathcal{G}u_n^h\, \mathcal{G}z_n^h \, d\boldsymbol{y}\, d\boldsymbol{x} = \int_{\omega_n} f_n\, z_n^h\, d\boldsymbol{x} \qquad \int_{\Omega_l} \nabla u_l^h \nabla z_l^h \, d\boldsymbol{x} = \int_{\Omega_l} f_l\, z_l^h\, d\boldsymbol{x}$$

IS THE SOLUTION UNIQUE?

Discrete reduced functional:

$$J_h(\theta_n^h, \theta_l^h) = \frac{1}{2}\|\underbrace{v_n^h(\theta_n^h) - v_l^h(\theta_l^h)}\|_{0,\Omega_o}^2 + \left(u_n^{h0} - u_l^{h0}, v_n^h(\theta_n^h) - v_l^h(\theta_l^h)\right)_{0,\Omega_o}$$

$$Q_h(\theta_n^h, \theta_l^h; \theta_n^h, \theta_l^h) = \|(\theta_n^h, \theta_l^h)\|_{h*}$$

control space **complete** wrt to the energy norm

Lemma: The discrete reduced space problem has a **unique** solution in the discrete control space

Key results: • strong discrete Cauchy-Schwarz inequality

$$|(v_n^h(\sigma_n^h), v_l^h(\sigma_l^h))_{0,\Omega_o}| < \delta\|v_n^h(\sigma_n^h)\|_{0,\Omega_o}\, \|v_l^h(\sigma_l^h)\|_{0,\Omega_o}, \quad \delta < 1$$

• **inner product** in the discrete control space

$$\int_{\Omega_o} \left(v_n^h(\sigma_n^h) - v_l^h(\sigma_l^h)\right)\left(v_n^h(\mu_n^h) - v_l^h(\mu_l^h)\right) := ((\sigma_n^h, \sigma_l^h), (\mu_n^h, \mu_l^h))_{h,*}$$

CONVERGENCE ANALYSIS

Approximation error (from 2nd Strang's lemma)

$$\|(\theta_n^* - \theta_n^{h*}, \theta_l^* - \theta_l^{h*})\|_{h*} \leq C_n h_n^{p_n+t} + C_l h_l^{p_l+1}$$

by using **equivalence** of norms

$$\|(\theta_n^* - \theta_n^{h*}, \theta_l^* - \theta_l^{h*})\|^2_{L^2 \times H^{\frac{1}{2}}} \leq K_n h_n^{2(p_n+t)} + K_l h_l^{2p_l+1}$$

we lose $\frac{1}{2}$ order

PRELIMINARY TEST – 1D

Accuracy tests

	ε	h	$e(u_n)$	rate	$e(u_l)$	rate	$e(\theta_n)$	rate
quadratic $u_n = u_l = x^2$	0.065	2^{-3}	2.36e-03	-	2.62e-03	-	6.52e-04	-
		2^{-4}	7.54e-04	1.65	7.12e-04	1.88	1.78e-04	1.87
		2^{-5}	1.88e-04	2.00	1.78e-04	2.00	4.45e-05	2.00
		2^{-6}	4.67e-05	2.01	4.44e-05	2.00	1.11e-05	2.00
		2^{-7}	1.14e-05	2.04	1.10e-05	2.01	2.76e-06	2.01
cubic $u_n = u_l = x^3$	0.065	2^{-3}	9.70e-03	-	2.95e-02	-	4.86e-03	-
		2^{-4}	2.68e-03	1.86	7.54e-03	1.97	1.20e-03	2.01
		2^{-5}	7.02e-04	1.93	1.90e-03	1.99	3.11e-04	1.95
		2^{-6}	1.78e-04	1.98	4.76e-04	2.00	7.89e-05	1.98
		2^{-7}	4.48e-05	1.99	1.19e-04	2.00	1.99e-05	1.98

NONLOCAL VECTOR CALCULUS

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- generalization of the classical vector calculus to nonlocal operators
- allows us to study nonlocal diffusion similarly to the classical, local, counterpart
- based on the concept of nonlocal fluxes

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Nonlocal operators acting on $u(\boldsymbol{x})\colon \mathbb{R}^d \to \mathbb{R}$ and $\boldsymbol{\nu}(\boldsymbol{x},\boldsymbol{y})\colon \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$

- divergence of $\boldsymbol{\nu}$: $\mathcal{D}\big(\boldsymbol{\nu}\big)(\boldsymbol{x}) = \displaystyle\int_{\mathbb{R}^n} \big(\boldsymbol{\nu}(\boldsymbol{x},\boldsymbol{y}) + \boldsymbol{\nu}(\boldsymbol{y},\boldsymbol{x})\big) \cdot \boldsymbol{\alpha}(\boldsymbol{x},\boldsymbol{y})\, d\boldsymbol{y}$
- gradient of u: $\mathcal{G}\big(u\big)(\boldsymbol{x},\boldsymbol{y}) = \big(u(\boldsymbol{y}) - u(\boldsymbol{x})\big)\boldsymbol{\alpha}(\boldsymbol{x},\boldsymbol{y})$
- nonlocal diffusion of u: $\mathcal{L}u(\boldsymbol{x}) = \mathcal{D}(\mathcal{G}u(\boldsymbol{x}))$

$$\mathcal{L}u(\boldsymbol{x}) = 2\int\big(u(\boldsymbol{y}) - u(\boldsymbol{x})\big)\, \boldsymbol{\alpha}(\boldsymbol{x},\boldsymbol{y}) \cdot \boldsymbol{\alpha}(\boldsymbol{x},\boldsymbol{y})\, d\boldsymbol{y}$$

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- allows us to study nonlocal diffusion similarly to the classical, local, counterpart
- based on the concept of nonlocal fluxes

Nonlocal operators acting on $u(\boldsymbol{x})\colon \mathbb{R}^d \to \mathbb{R}$ and $\boldsymbol{\nu}(\boldsymbol{x},\boldsymbol{y})\colon \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$

- divergence of $\boldsymbol{\nu}$: $\mathcal{D}\big(\boldsymbol{\nu}\big)(\boldsymbol{x}) = \displaystyle\int_{\mathbb{R}^n} \big(\boldsymbol{\nu}(\boldsymbol{x},\boldsymbol{y}) + \boldsymbol{\nu}(\boldsymbol{y},\boldsymbol{x})\big) \cdot \boldsymbol{\alpha}(\boldsymbol{x},\boldsymbol{y})\, d\boldsymbol{y}$
- gradient of u: $\mathcal{G}\big(u\big)(\boldsymbol{x},\boldsymbol{y}) = \big(u(\boldsymbol{y}) - u(\boldsymbol{x})\big)\boldsymbol{\alpha}(\boldsymbol{x},\boldsymbol{y})$
- nonlocal diffusion of u: $\mathcal{L}u(\boldsymbol{x}) = \mathcal{D}(\mathcal{G}u(\boldsymbol{x}))$

$$\mathcal{L}u(\boldsymbol{x}) = 2\int \big(u(\boldsymbol{y}) - u(\boldsymbol{x})\big)\, \underline{\boldsymbol{\alpha}(\boldsymbol{x},\boldsymbol{y}) \cdot \boldsymbol{\alpha}(\boldsymbol{x},\boldsymbol{y})}\, d\boldsymbol{y}$$

$$\mathcal{L}u(\boldsymbol{x}) = 2\int \big(u(\boldsymbol{y}) - u(\boldsymbol{x})\big)\, \underline{\gamma(\boldsymbol{x},\boldsymbol{y})}\, d\boldsymbol{y}$$