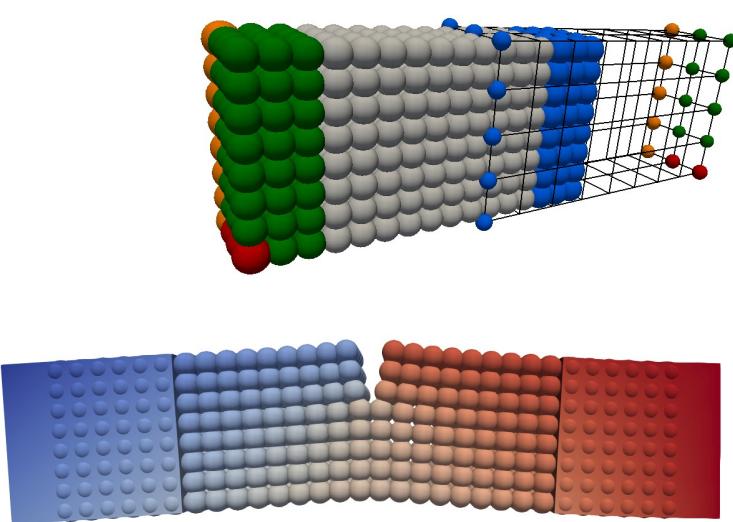


A COUPLING STRATEGY FOR CLASSICAL AND NONLOCAL ELASTICITY MODELS



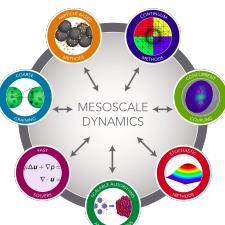
Nonlocal School on Fractional Equations
Iowa State University, August 17–19, 2017

Marta D'Elia, P. Bochev, D. Littlewood, M. Perego

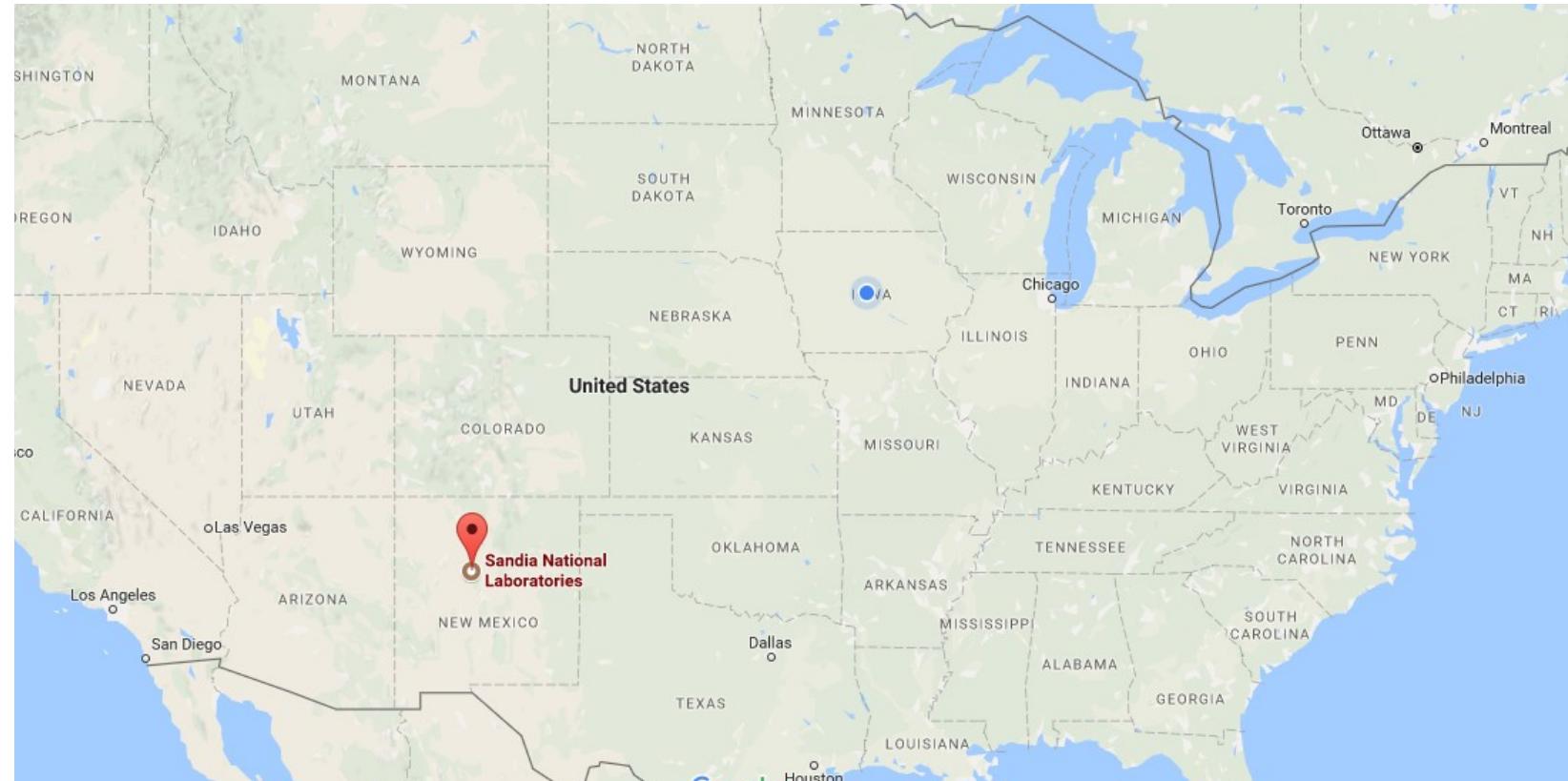


Sandia National Laboratories

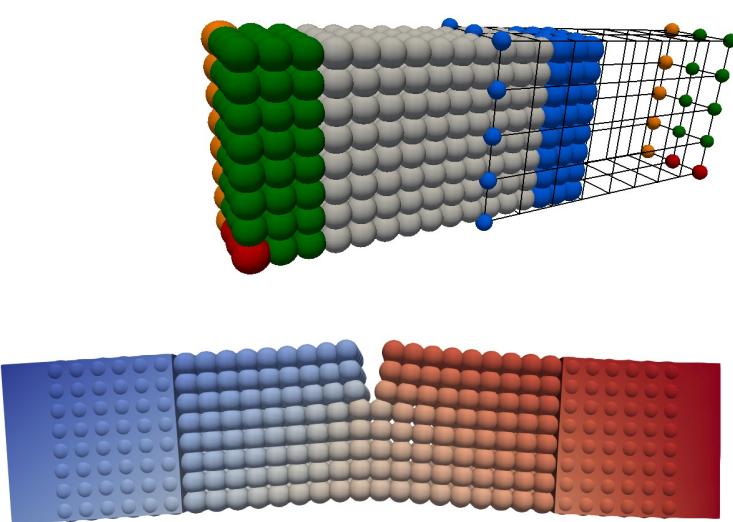
Sandia National Labs, NM – Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.







A COUPLING STRATEGY FOR CLASSICAL AND NONLOCAL ELASTICITY MODELS



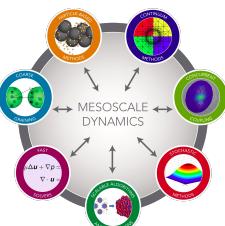
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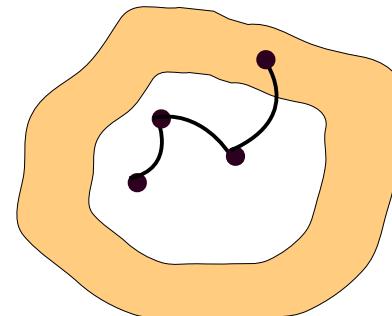
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NONLOCAL MODELS

what I use nonlocal models for

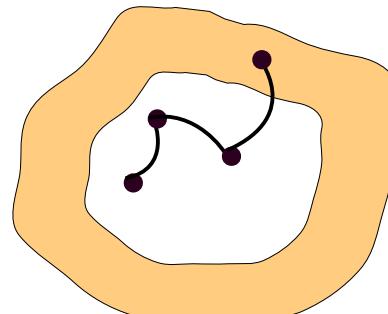
- peridynamic model for mechanics
- jump processes/fractional operators
- image processing



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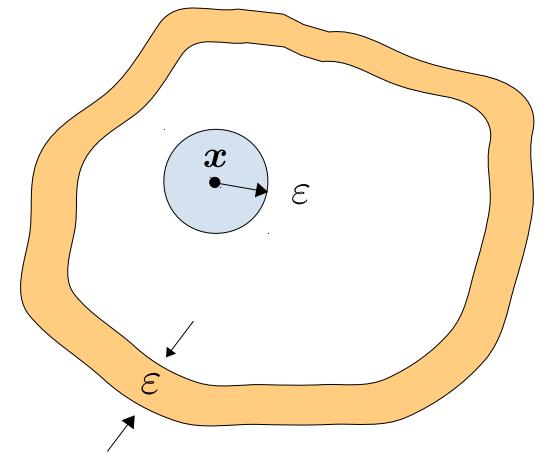


how do they look like?

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

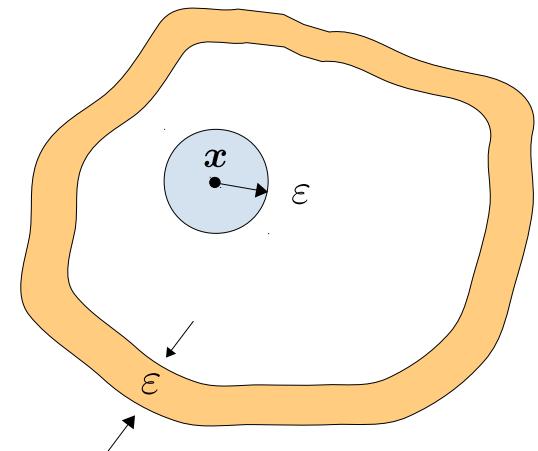
NONLOCAL MODELS

- interactions can occur at distance, but are localized
- used in many scientific and engineering applications, where the material dynamics depends on microstructure



NONLOCAL MODELS

- interactions can occur at distance, but are localized
- used in many scientific and engineering applications, where the material dynamics depends on microstructure
- example: nonlocal continuum mechanics theories, e.g. **peridynamics**[1] and physics-based **nonlocal elasticity**[2] which can model fractures and material failures



ductile fracture,
Wikipedia

[1] S.Silling, R.B.Lehoucq, Advances in Applied Mechanics, Elsevier, 2010.

[2] M.Di Paola, G.Failla, and M.Zingales, Journal of Elasticity, 2009.

NONLOCAL MODELS

- facts:**
- the **nonlocal vector calculus** allows us to study nonlocal problems **similarly** to the local counterpart
 - we have several discretization schemes and **numerical convergence** results for finite element approximations

NONLOCAL MODELS

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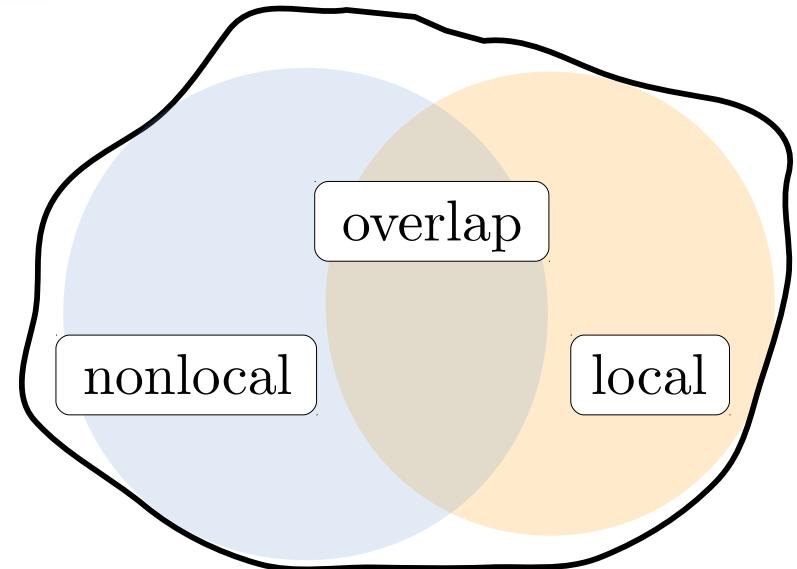
- we have several discretization schemes and **numerical convergence** results for finite element approximations

challenges: • the numerical solution might be **prohibitively expensive**

- prescription of nonlocal “boundary conditions” is not straightforward

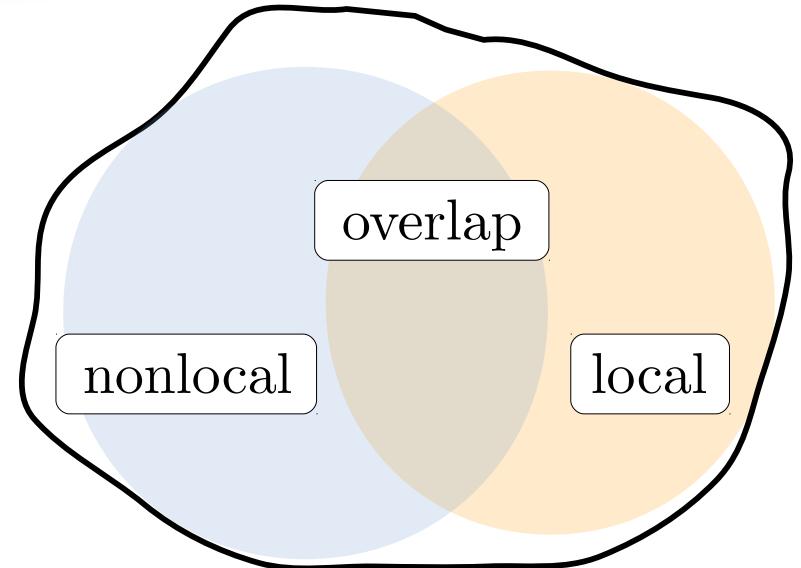
COUPLING

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



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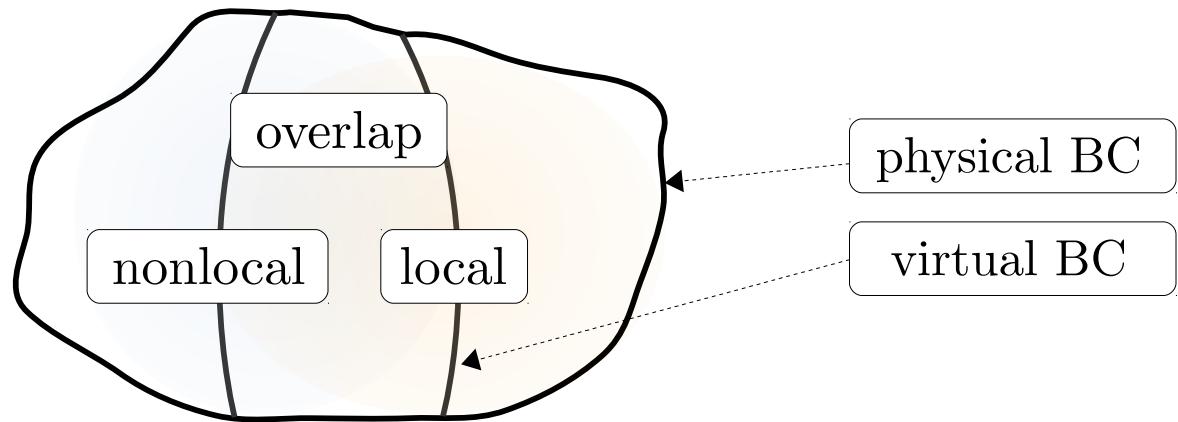


Local-Nonlocal coupling

- (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 **trace theorems**

COUPLING

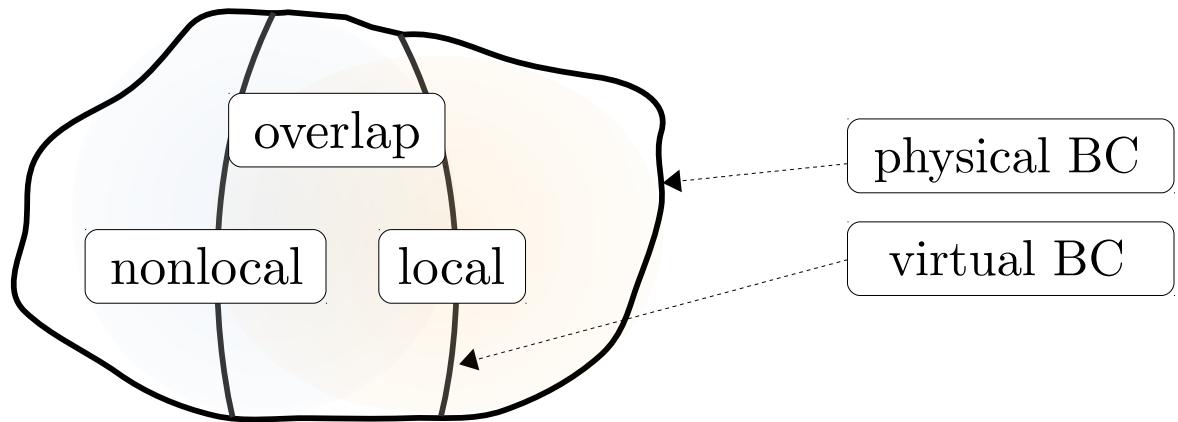
Our strategy split the computational domain in a local and a nonlocal domain and **couple** the models at the interfaces or overlapping regions [*]



[*] Du 2000,2001; Gunzburger 1999,2000; Lions 2000;
Bochev 2009, 2011, 2016; Discacciati 2013; Olson 2014.

COUPLING

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



$$\min_{\mathbf{u}_n, \mathbf{u}_l, \boldsymbol{\nu}_n, \boldsymbol{\nu}_l} \mathcal{J}(\mathbf{u}_n, \mathbf{u}_l) = \frac{1}{2} \|\mathbf{u}_n - \mathbf{u}_l\|_{*,\text{overlap}}^2$$

$$\text{s.t. } \left\{ \begin{array}{ll} -\mathcal{L}_n \mathbf{u}_n = \mathbf{b} & \text{nonlocal} \\ \mathbf{u}_n = \mathbf{g} & \text{physical BC} \\ \mathbf{u}_n = \boldsymbol{\nu}_n & \text{virtual BC} \end{array} \right. \quad \left\{ \begin{array}{ll} -\mathcal{L}_l \mathbf{u}_l = \mathbf{b} & \text{local domain} \\ \mathbf{u}_l = \mathbf{g} & \text{physical BC} \\ \mathbf{u}_l = \boldsymbol{\nu}_l & \text{virtual BC} \end{array} \right.$$

COUPLING

Contribution: design a local-to-nonlocal coupling method that

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

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Novelty: design a method that differs fundamentally from previous strategies
reversing the roles of coupling conditions and models

- coupling conditions = optimization objective
- models = optimization constraints

OUTLINE

- Nonlocal Vector Calculus
- Nonlocal diffusion
 - 1. formulation and analysis
 - 2. finite dimensional approximation
 - 3. numerical results
- Static peridynamics
 - 1. formulation and finite dimensional approximation
 - 2. numerical results

A NONLOCAL VECTOR CALCULUS

- Q. Du, M.D. Gunzburger, R. Lehoucq, and K. Zhou, Analysis and approximation of nonlocal diffusion problems with volume constraints.

SIAM Review, 54, 667–696, 2012

- Q. Du, M. Gunzburger, R. Lehoucq, and K. Zhou, A nonlocal vector calculus, nonlocal volume-constrained problems, and nonlocal balance laws.

Math. Model. Meth. Appl. Sci, 23, 493–540, 2013

NONLOCAL VECTOR CALCULUS

- generalization of the classical vector calculus to nonlocal operators
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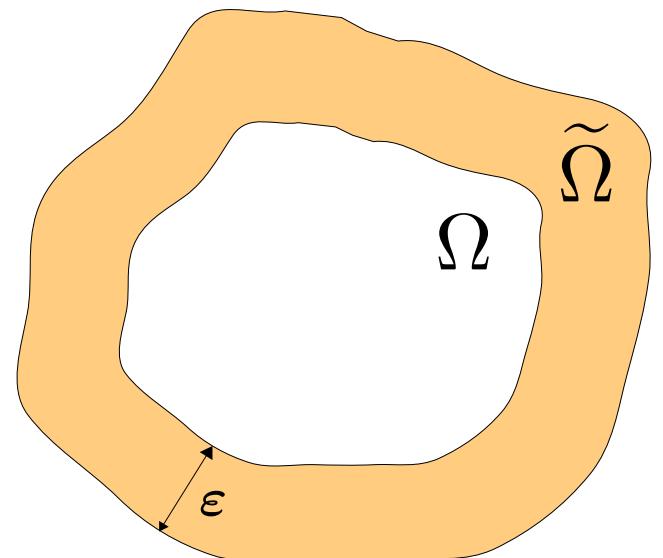
Nonlocal operators: $u(x)$, $\nu(x, y)$, $\alpha(x, y) = -\alpha(y, x)$

- divergence of ν : $\mathcal{D}(\nu)(\mathbf{x}) = \int (\nu(\mathbf{x}, \mathbf{y}) + \nu(\mathbf{y}, \mathbf{x})) \cdot \boldsymbol{\alpha}(\mathbf{x}, \mathbf{y}) d\mathbf{y}$
 - gradient of u : $\mathcal{G}(u)(\mathbf{x}, \mathbf{y}) = (u(\mathbf{y}) - u(\mathbf{x})) \boldsymbol{\alpha}(\mathbf{x}, \mathbf{y})$
 - nonlocal diffusion of u : $\mathcal{L}u(\mathbf{x}) = \mathcal{D}(\mathcal{G}u(\mathbf{x}))$

NONLOCAL VECTOR CALCULUS

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

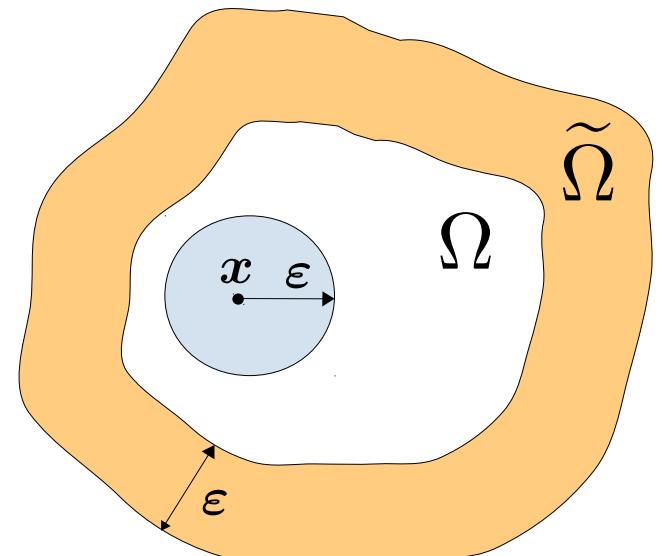
$$\tilde{\Omega} = \{ \mathbf{y} \in \mathbb{R}^d \setminus \Omega : \alpha(\mathbf{x}, \mathbf{y}) \neq 0, \mathbf{x} \in \Omega \},$$



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Kernel: we assume

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

$$B_\varepsilon(\mathbf{x}) = \{ \mathbf{y} \in \Omega \cup \tilde{\Omega} : |\mathbf{x} - \mathbf{y}| \leq \varepsilon, \mathbf{x} \in \Omega \}$$

NONLOCAL VECTOR CALCULUS

energy norm and energy space

$$|||v|||_{\Omega^+}^2 = \int_{\Omega^+} \int_{\Omega^+} \mathcal{G}v \mathcal{G}v \, dy \, dx$$

semi-energy norm

$$V(\Omega^+) = \{v \in L^2(\Omega^+) : |||v|||_{\Omega^+} < \infty\}$$

energy space

$$V_0(\Omega^+) = \left\{ v \in V(\Omega^+) : v = 0 \text{ in } \tilde{\Omega} \right\}$$

constrained energy space

NONLOCAL VECTOR CALCULUS

kernels and equivalence of spaces

case 1: $\frac{\gamma_1}{|\mathbf{x} - \mathbf{y}|^{n+2s}} \leq \gamma(\mathbf{x}, \mathbf{y}) \leq \frac{\gamma_2}{|\mathbf{x} - \mathbf{y}|^{n+2s}}$ $\Rightarrow V_0(\Omega^+) \cong H^s(\Omega^+)$

case 2: $\gamma_3 \leq \int_{\Omega^+ \cap B_\varepsilon(\mathbf{x})} \gamma(\mathbf{x}, \mathbf{y}) d\mathbf{y} \quad \forall \mathbf{x} \in \Omega$
 $\Rightarrow V_0(\Omega^+) \cong L^2(\Omega^+)$

$$\int_{\Omega^+ \cap B_\varepsilon(\mathbf{x})} \gamma^2(\mathbf{x}, \mathbf{y}) d\mathbf{y} \leq \gamma_4 \quad \forall \mathbf{x} \in \Omega$$

NONLOCAL VECTOR CALCULUS

Variational form of a diffusion problem

strong form:
$$\begin{cases} -\mathcal{L}u = f & \mathbf{x} \in \Omega \\ u = 0 & \mathbf{x} \in \tilde{\Omega}, \end{cases}$$

weak form: $\int_{\Omega} \mathcal{L}u v d\mathbf{x} = \int_{\Omega} f v d\mathbf{x} \quad \forall v \in V_0$

integration by parts

$$\int_{\Omega} \int_{\Omega} \mathcal{G}u \mathcal{G}v d\mathbf{y} d\mathbf{x} = \int_{\Omega} f v d\mathbf{x} \quad \forall v \in V_0$$



$$\int_{\Omega} \int_{\Omega} (u(\mathbf{x}) - u(\mathbf{y})) (v(\mathbf{x}) - v(\mathbf{y})) \gamma(\mathbf{x}, \mathbf{y}) d\mathbf{y} d\mathbf{x}$$

THE LtN OPTIMIZATION PROBLEM

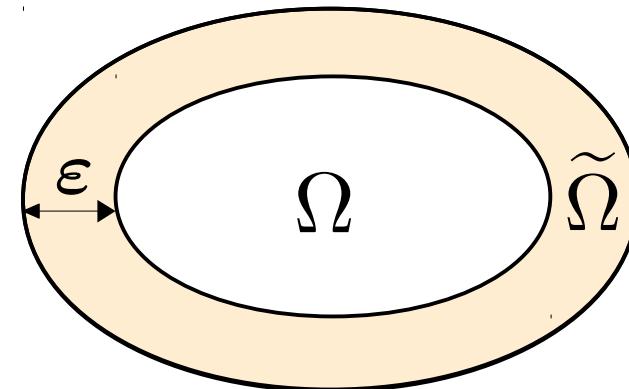
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MODEL PROBLEMS (Poisson – Dirichlet)

The nonlocal problem

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

where $\sigma_n \in \tilde{V}(\tilde{\Omega})$ and $f_n \in L^2(\Omega)$

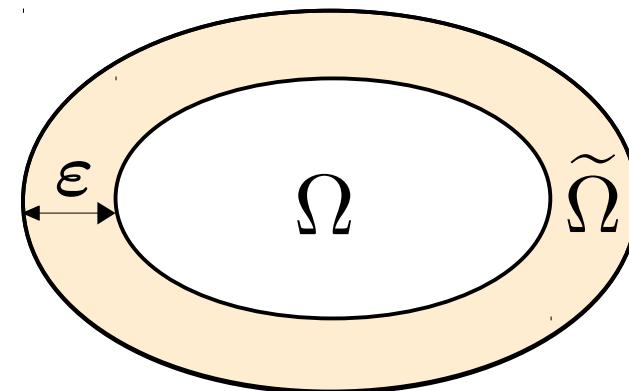


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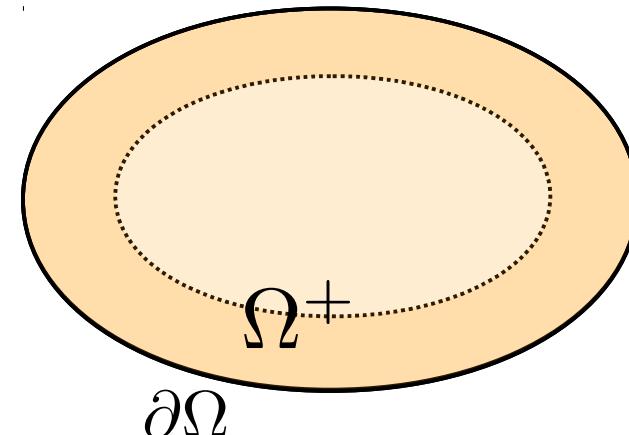
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The local problem: Poisson equation

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

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

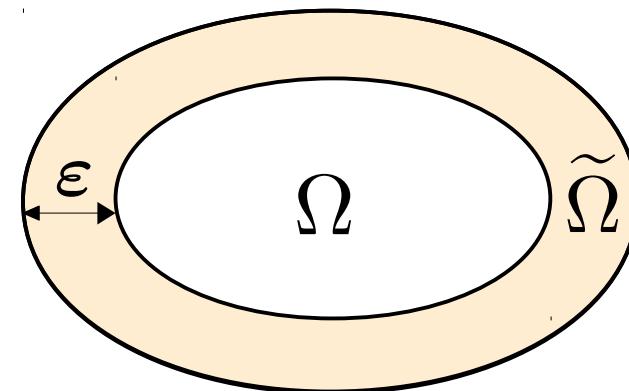


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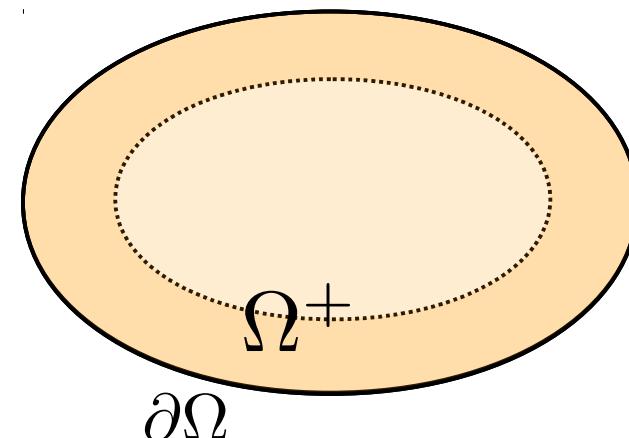


as $\varepsilon \rightarrow 0$
converges to

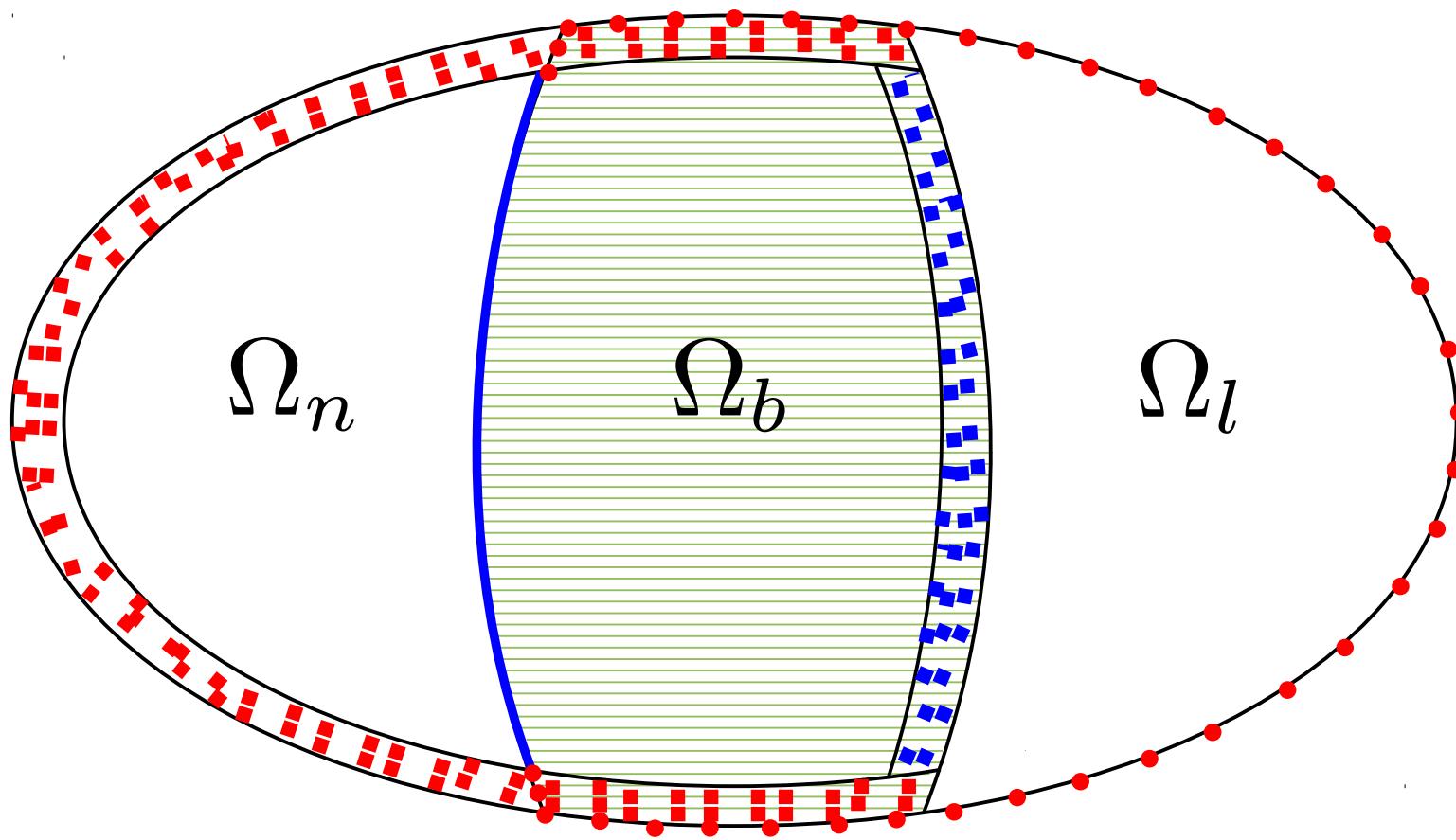
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LtN COUPLING



⋮ ⋮ ⋮ $\tilde{\Omega}_i$

⋮ ⋮ ⋮ $\tilde{\Omega}_c$

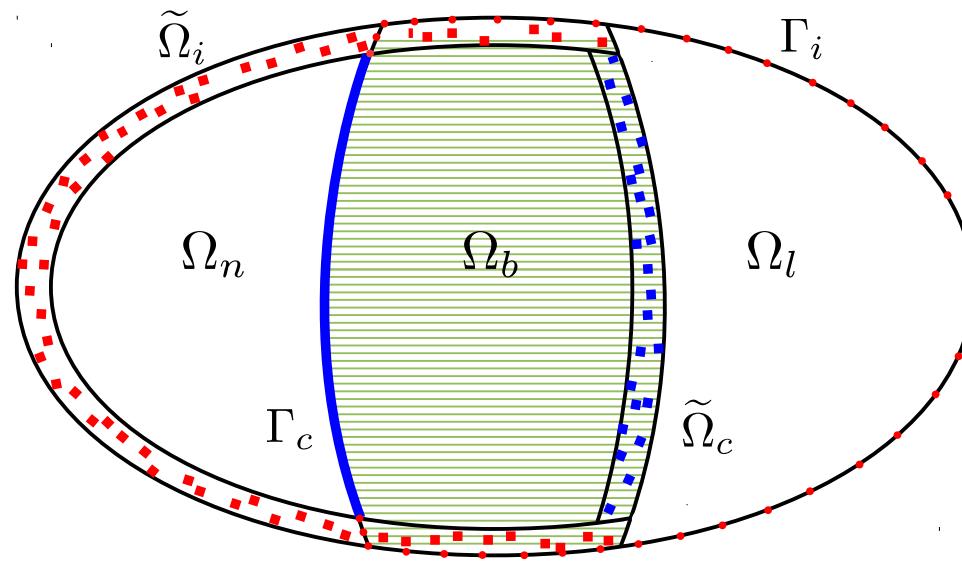
Γ_i • — • — •

Γ_c —

LtN COUPLING

State equations:

$$\left\{ \begin{array}{l} -\mathcal{L}u_n = f_n \quad \mathbf{x} \in \Omega_n \\ u_n = \theta_n \quad \mathbf{x} \in \tilde{\Omega}_c \\ u_n = 0 \quad \mathbf{x} \in \tilde{\Omega}_i \end{array} \right. \quad \left\{ \begin{array}{l} -\Delta u_l = f_l \quad \mathbf{x} \in \Omega_l \\ u_l = \theta_l \quad \mathbf{x} \in \Gamma_c \\ u_l = 0 \quad \mathbf{x} \in \Gamma_i. \end{array} \right.$$



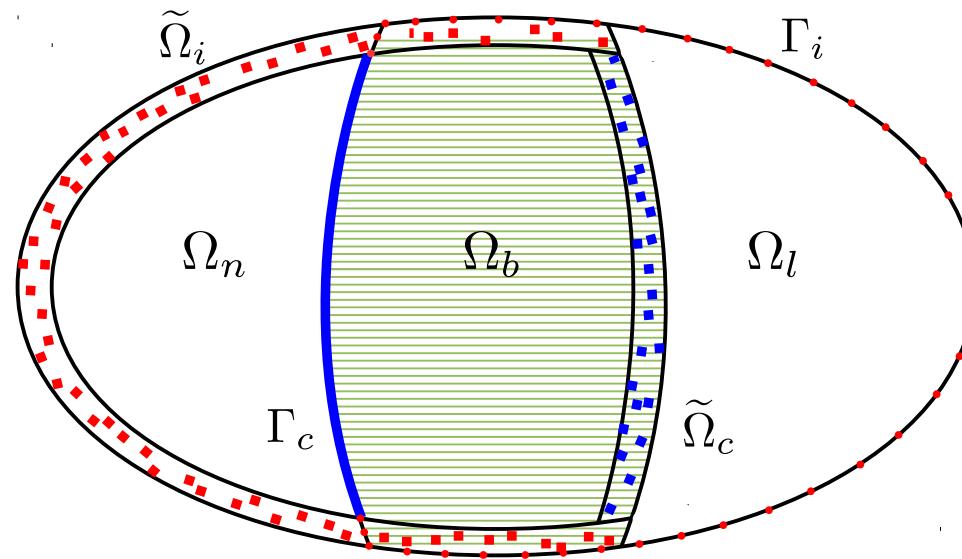
LtN COUPLING

Optimization problem:

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

s.t.
$$\begin{cases} -\mathcal{L}u_n &= f_n & \mathbf{x} \in \Omega_n \\ u_n &= \theta_n & \mathbf{x} \in \tilde{\Omega}_c \\ u_n &= 0 & \mathbf{x} \in \tilde{\Omega}_i \end{cases} \quad \begin{cases} -\Delta u_l &= f_l & \mathbf{x} \in \Omega_l \\ u_l &= \theta_l & \mathbf{x} \in \Gamma_c \\ u_l &= 0 & \mathbf{x} \in \Gamma_i. \end{cases}$$

$(\theta_n, \theta_l) \in \Theta_n \times \Theta_l$: control variables



LtN COUPLING

LtN solution • optimal solution: $(\theta_n^*, \theta_l^*) \in \Theta_n \times \Theta_l$

• LtN solution: $u^* = \begin{cases} u_n^*(\theta_n^*) & x \in \Omega_n \\ u_l^*(\theta_l^*) & x \in \Omega_l \setminus \Omega_b \end{cases}$

IS THE SOLUTION UNIQUE?

Reduced form:

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

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Solution splitting:

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

harmonic components v_n and v_l

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

homogeneous components u_n^0 and u_l^0

$$\begin{cases} -\mathcal{L}u_n^0 = f_n & \boldsymbol{x} \in \Omega_n \\ u_n^0 = 0 & \boldsymbol{x} \in \tilde{\Omega}_c \\ + \text{VC} \end{cases} \quad \text{and} \quad \begin{cases} -\Delta u_l^0 = f_l & \boldsymbol{x} \in \Omega_l \\ u_l^0 = 0 & \boldsymbol{x} \in \Gamma_c \\ + \text{BC} \end{cases}$$

IS THE SOLUTION UNIQUE?

Reduced functional:

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

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

IS THE SOLUTION UNIQUE?

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

Key result: $\int_{\Omega_b} (v_n(\sigma_n) - v_l(\sigma_l)) (v_n(\mu_n) - v_l(\mu_l)) dx := ((\sigma_n, \sigma_l), (\mu_n, \mu_l))_*$

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

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

defines a norm in the control variable space

FINITE DIMENSIONAL APPROXIMATION

- 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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FINITE ELEMENT DISCRETIZATIONS

1D simulations: discretize local and nonlocal models with FEM

- the discretized problem has a unique solution
- the method passes a patch test
- the convergence rate is optimal

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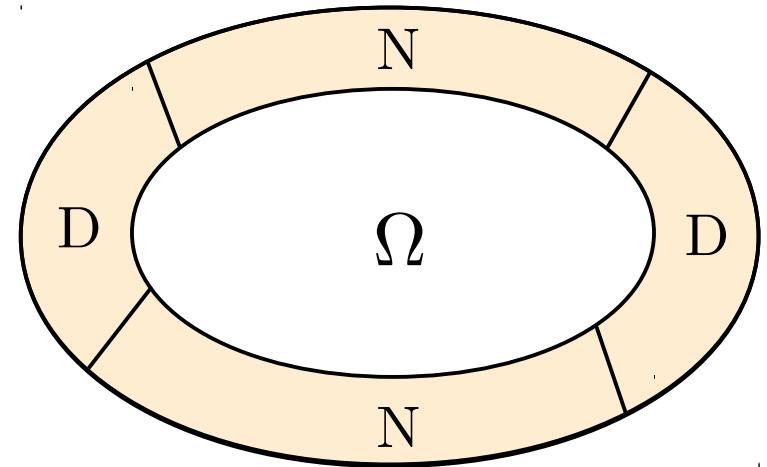
but the real world

- is not in 1D
- does not have Dirichlet conditions

MODEL PROBLEMS (Poisson – Dirichlet & Neumann)

The nonlocal problem

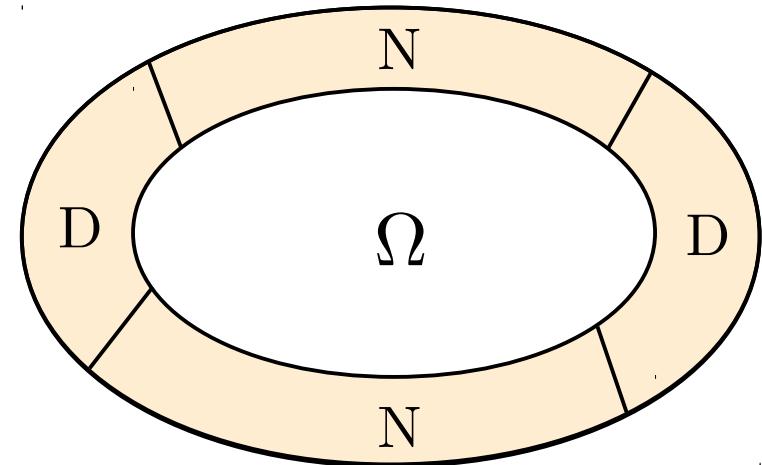
$$\begin{cases} -\mathcal{L}u_n = f_n & \mathbf{x} \in \Omega \\ u_n = \sigma_n & \mathbf{x} \in D \\ \mathcal{N}(\mathcal{G}u_n) = \eta_n & \mathbf{x} \in N \end{cases} \quad \begin{array}{l} \text{Dirichlet (D)} \\ \text{Neumann (N)} \end{array}$$



MODEL PROBLEMS (Poisson – Dirichlet & Neumann)

The nonlocal problem

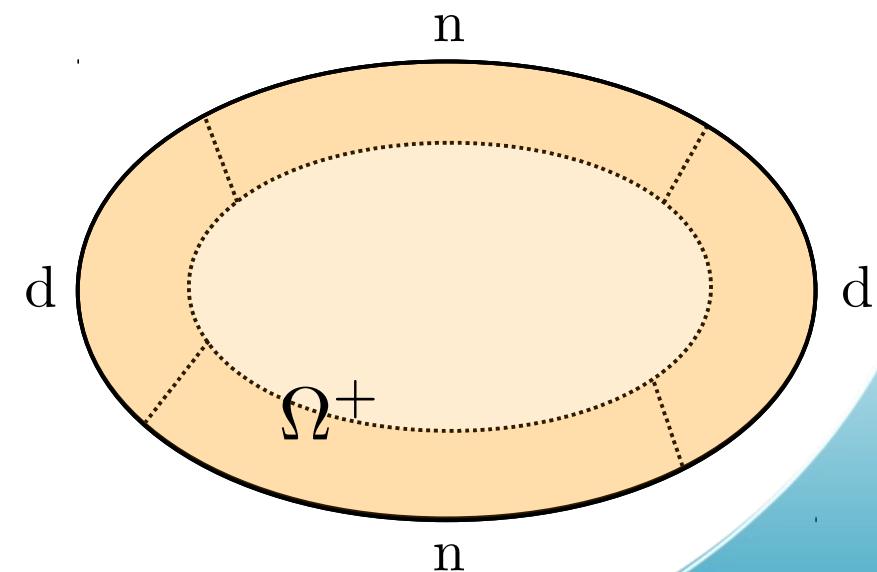
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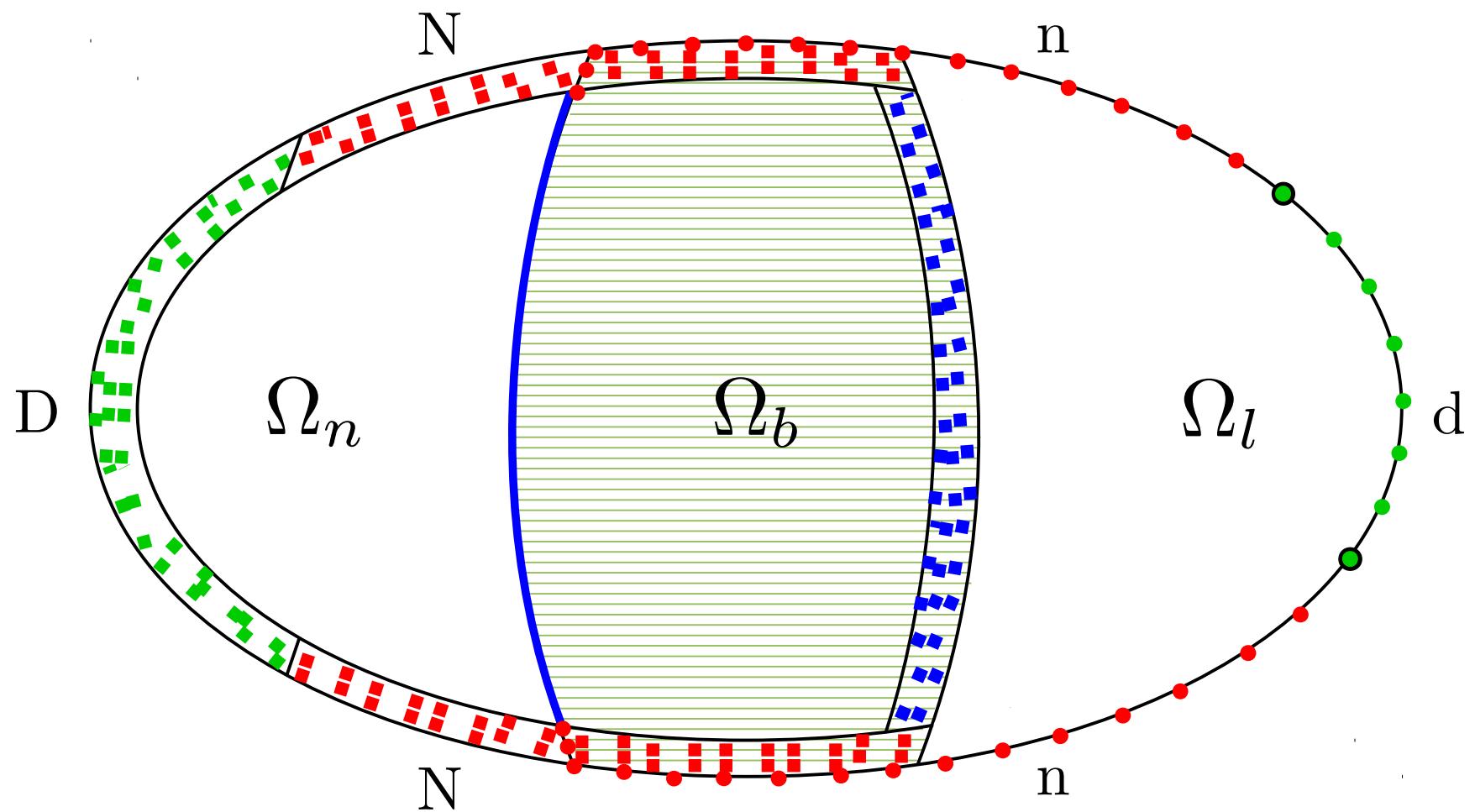
as $\varepsilon \rightarrow 0$
converges to

The local problem

$$\begin{cases} -\Delta u_l = f_l & \mathbf{x} \in \Omega^+ \\ u_l = \sigma_l & \mathbf{x} \in d \\ -\nabla u_l \cdot \mathbf{n} = \eta_l & \mathbf{x} \in n \end{cases} \quad \begin{array}{l} \text{Dirichlet (d)} \\ \text{Neumann (n)} \end{array}$$



COUPLING CONFIGURATION



Note: the Dirichlet-Neumann problem is well-posed.

THE DISCRETIZATION

Goal: exploit the flexibility of the method and use two **fundamentally different** discretization schemes for the local and the nonlocal models

$$\begin{cases} -\mathcal{L}u_n = f_n & \boldsymbol{x} \in \Omega_n \\ u_n = \theta_n & \boldsymbol{x} \in \tilde{\Omega}_c \\ +\text{VC} \end{cases}$$

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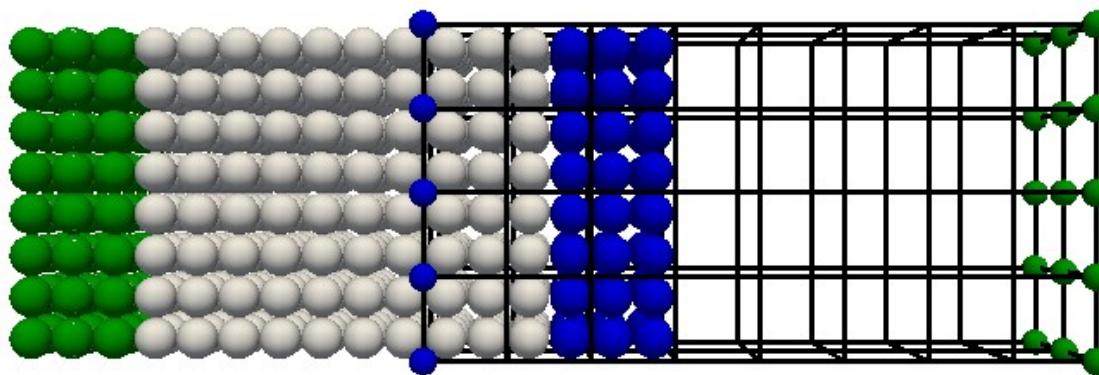
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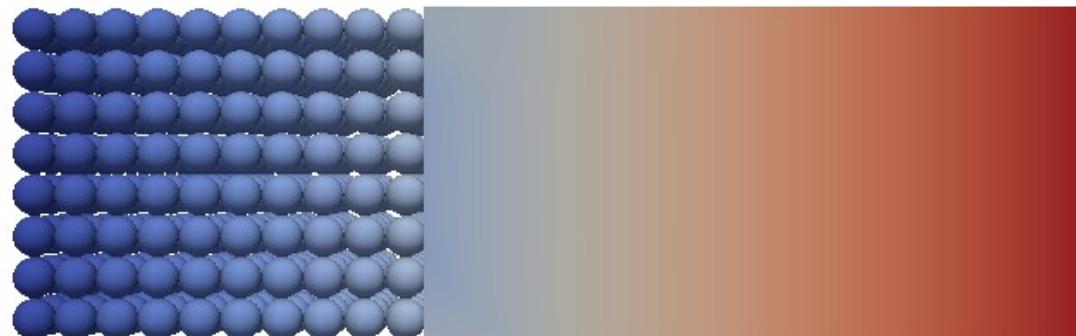


QUICK EXAMPLE



kernel: $\gamma(\mathbf{x}, \mathbf{y}) = \frac{3}{\pi\varepsilon^4} \frac{1}{|\mathbf{x} - \mathbf{y}|}, \quad |\mathbf{x} - \mathbf{y}| \leq \varepsilon$

analytic solution: $\mathbf{u} = (x, 0, 0)$, **linear** patch test



patch test

STATIC PERIDYNAMICS

- D. Littlewood, M. Perego, M. D'Elia, P. Bochev, A coupling approach for static peridynamics and classical elasticity, *in preparation*
- 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:

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

u: displacement field, **b**: given body force, **T**: force state field

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PD model: linearized linear peridynamic solid (LPS) model

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LPS equation: $-\mathcal{L}_{\text{LPS}}[\mathbf{u}](\mathbf{x}) = \mathbf{b}(\mathbf{x}) \quad \mathbf{x} \in \Omega_n, \quad \mathbf{u}(\mathbf{x}) = \mathbf{g}(\mathbf{x}) \quad \mathbf{x} \in \tilde{\Omega}_i$

THE LOCAL MODEL

Local equation: Navier-Cauchy model of linear elasticity

$$-\mathcal{L}_{\text{NC}}[\mathbf{u}](\mathbf{x}) = \mathbf{b}(\mathbf{x}), \text{ with}$$

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

- Note:**
- for a quadratic displacement field LPS = NC
 - for $\varepsilon \rightarrow 0$, **Peridynamics** → **Linear classical elasticity**

THE COUPLING STRATEGY

Optimization-based coupling

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

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Discretization:

local problem: variational form with FEM

nonlocal problem: strong form with mesh free method \rightarrow modified operator

$$L[\mathbf{x}_i] := \sum_{j \in \mathcal{N}_i} \{ \mathbf{T}[\mathbf{x}_i] \langle \mathbf{x}_j - \mathbf{x}_i \rangle - \mathbf{T}[\mathbf{x}_j] \langle \mathbf{x}_i - \mathbf{x}_j \rangle \} V_j^{(i)}$$

$$V_j^{(i)} = |B_\varepsilon(\mathbf{x}_i) \cap B_\varepsilon(\mathbf{x}_j)|$$

SOFTWARE*

Coupling Peridigm and Albany

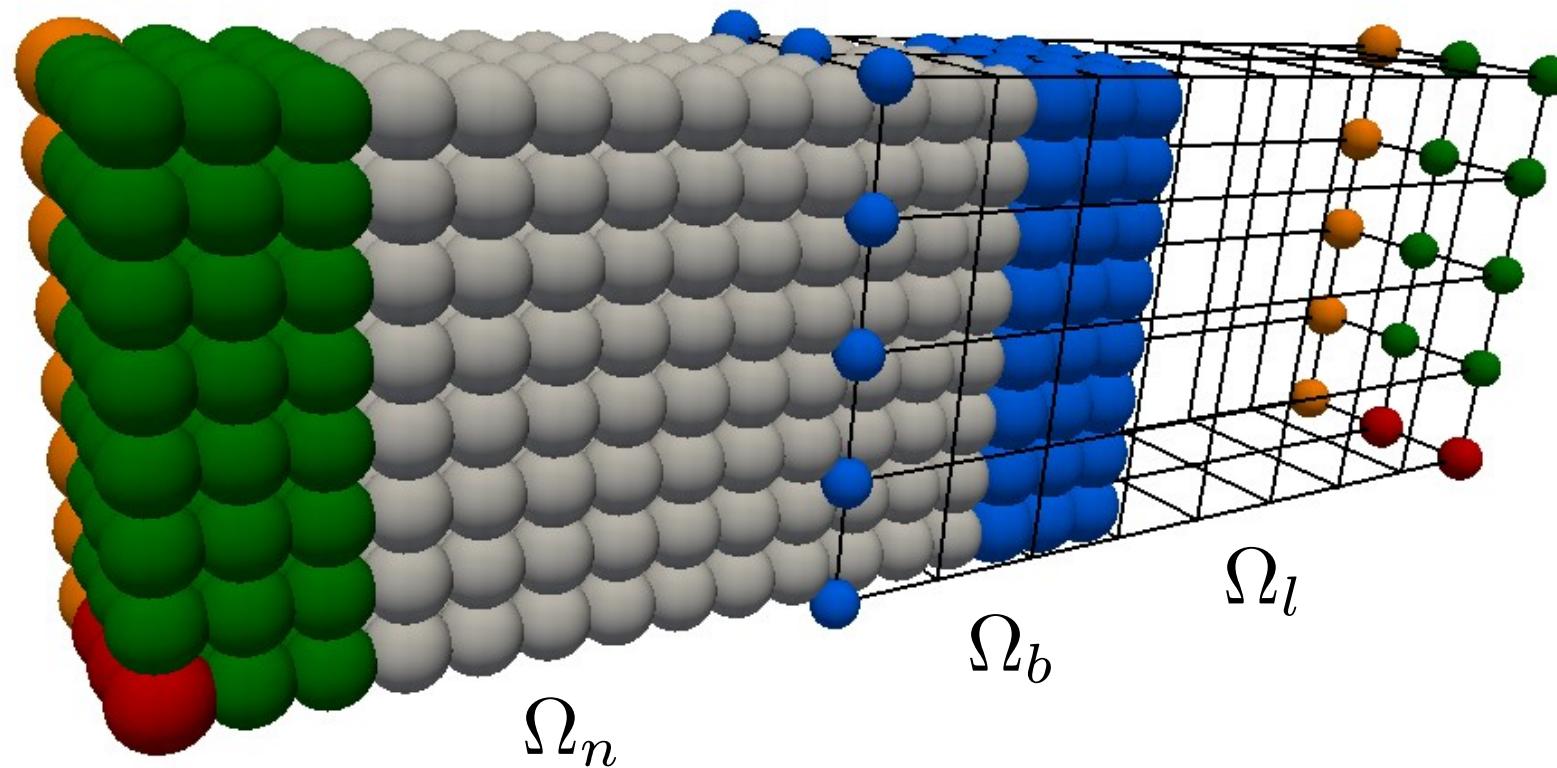


peridigm.sandia.gov

software.sandia.gov/albany/

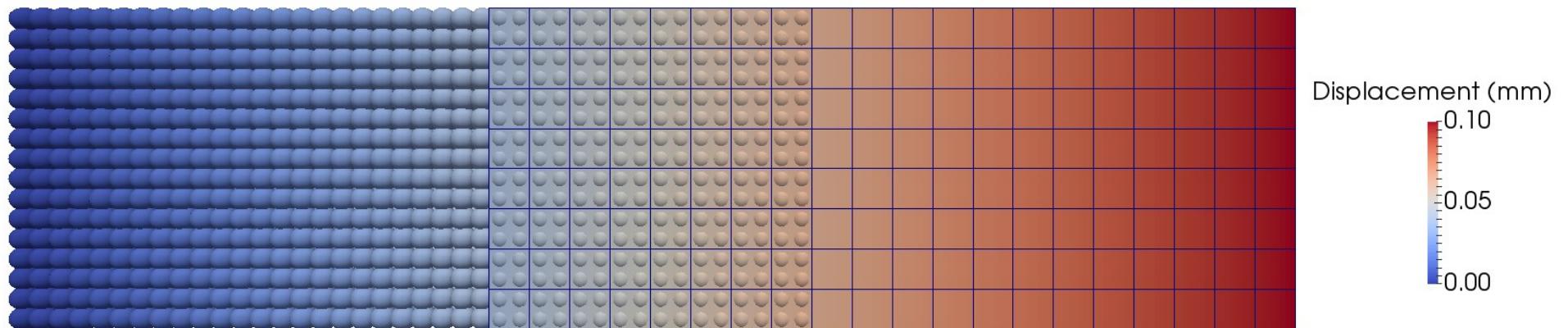
trilinos.org/packages/rol

THE GEOMETRY



THE PATCH TEST

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



$$\Omega_n$$

$$\Omega_b$$

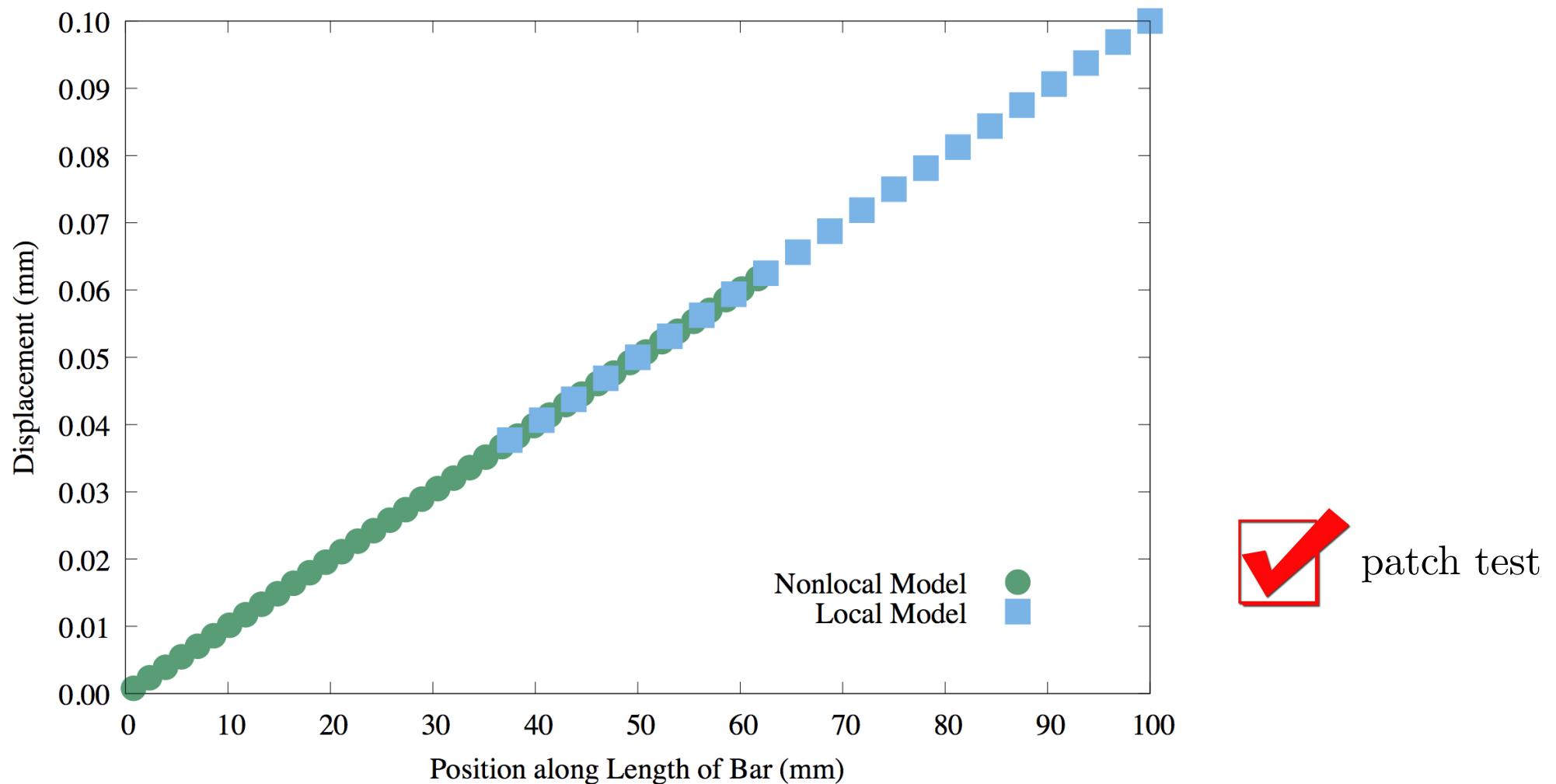
$$\Omega_l$$



patch test

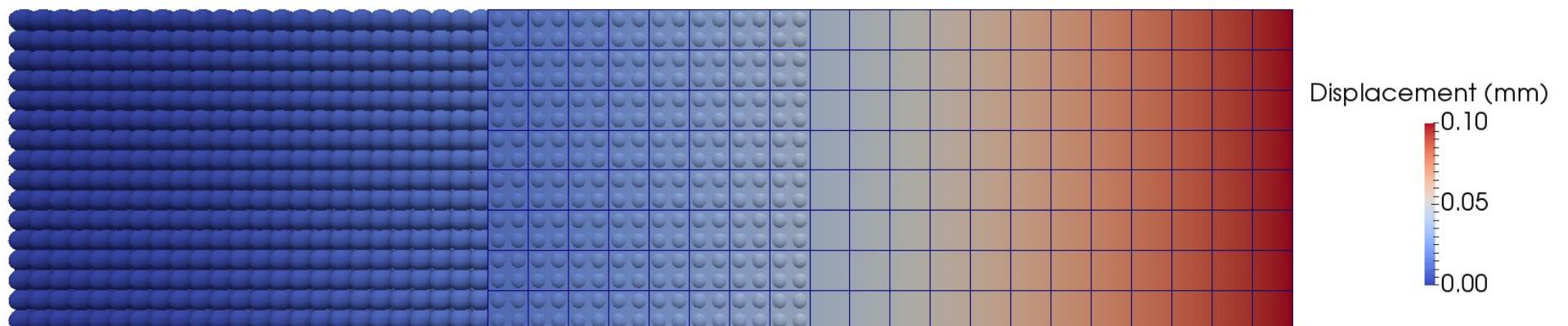
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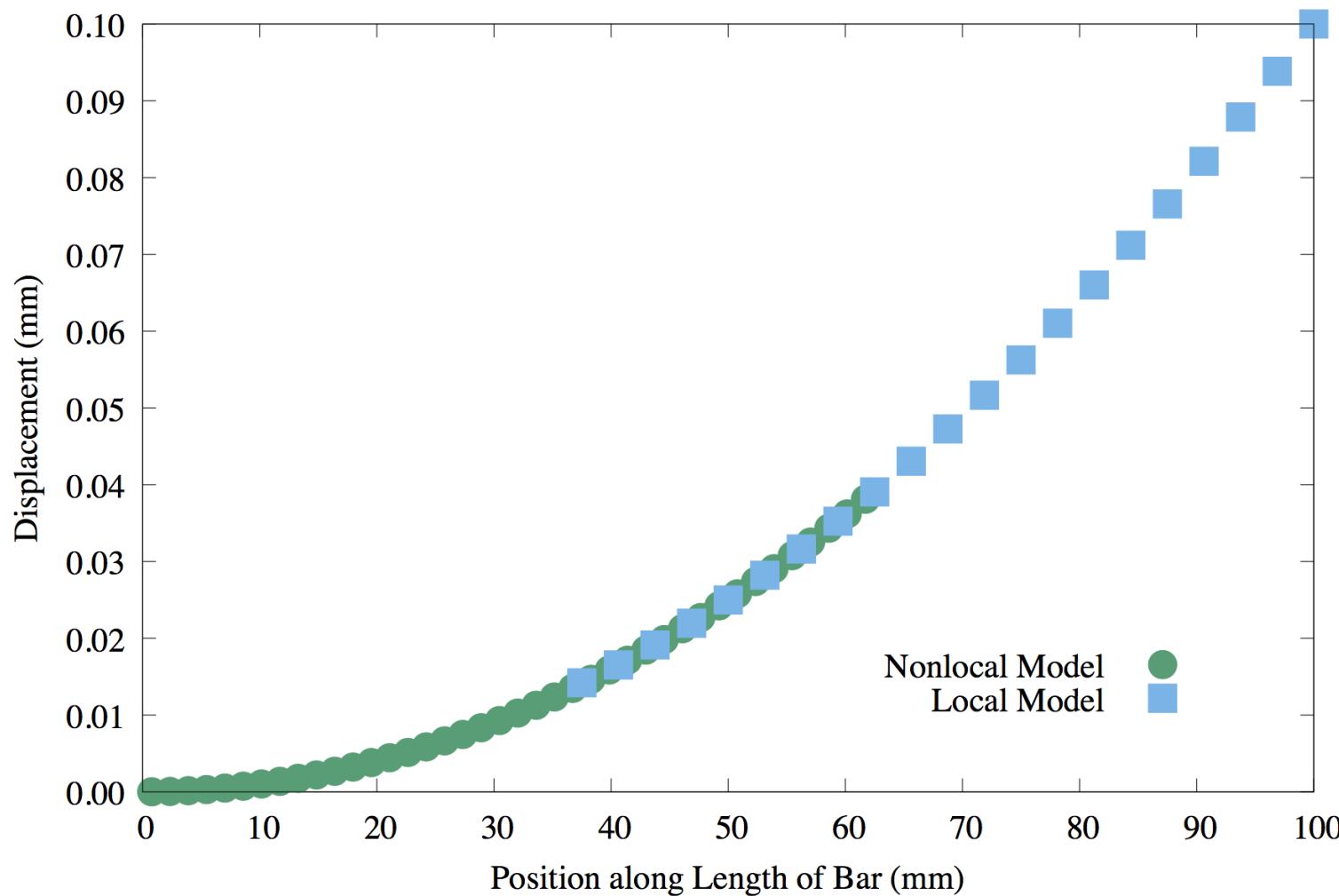
Analytic solution: $\mathbf{u} = 10^{-5}(x^2, 0, 0)$, **quadratic** patch test

 Ω_n Ω_b Ω_l 

patch test

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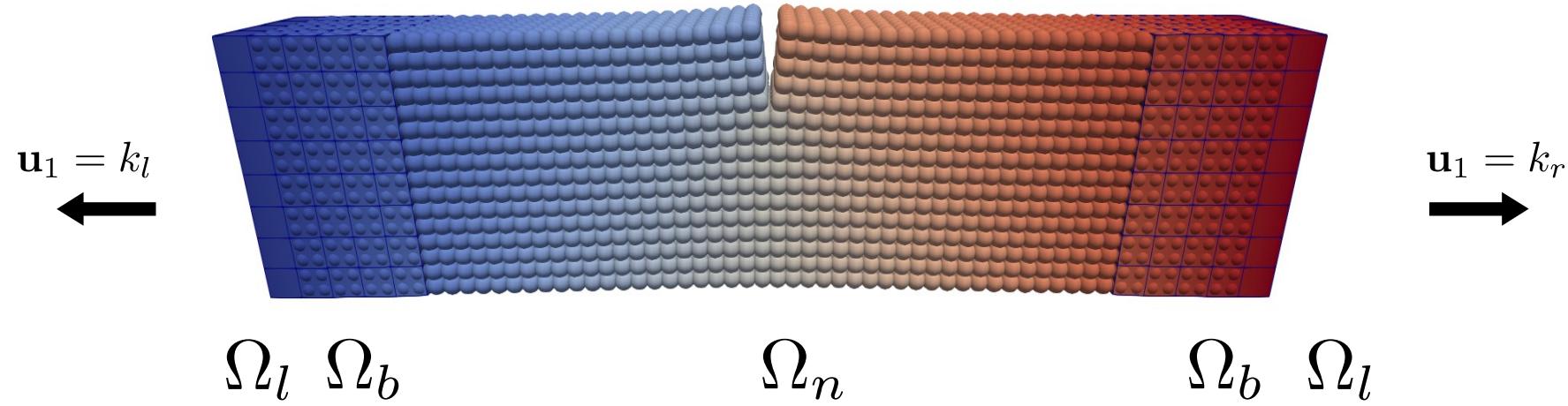
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patch test

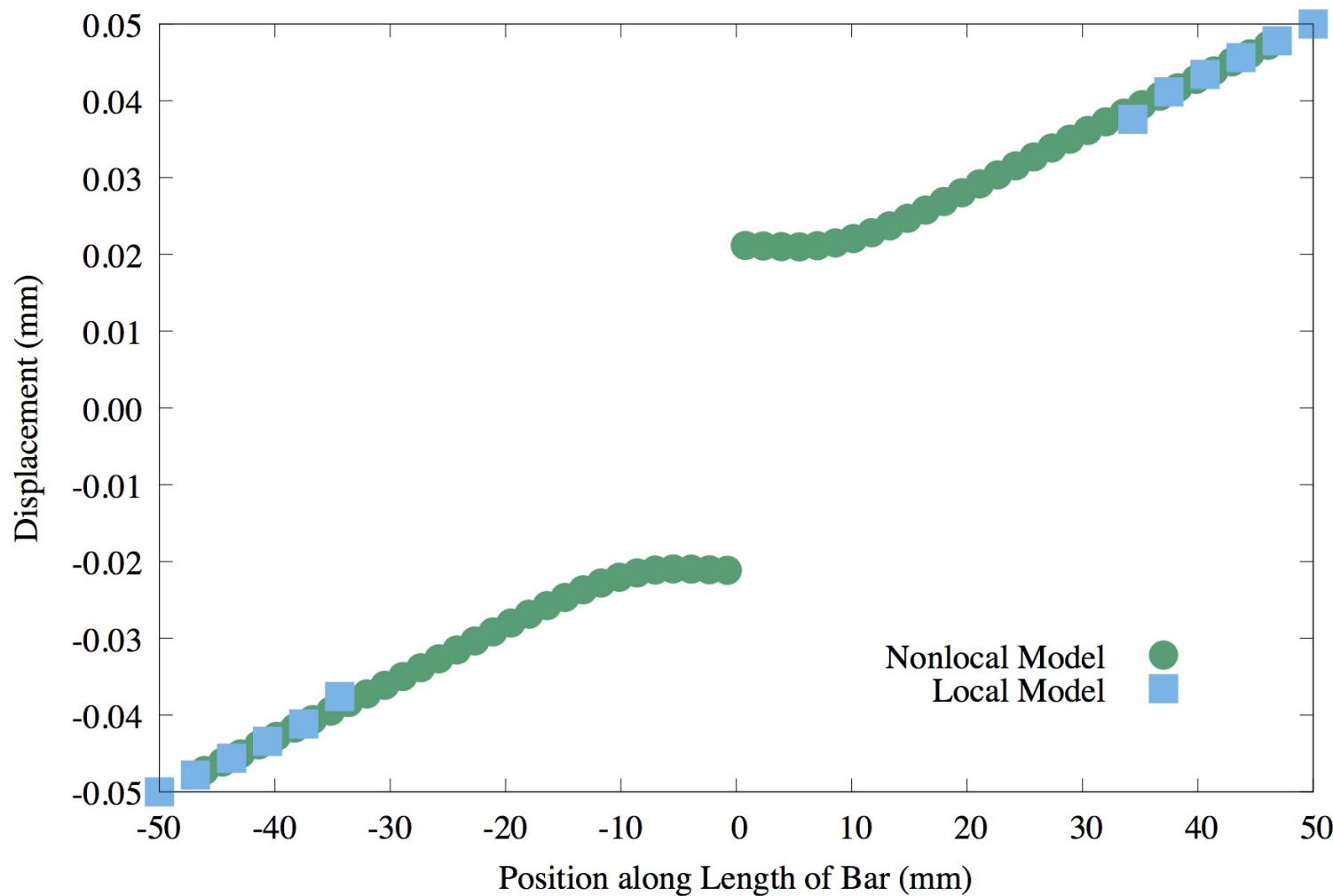
CRACK TEST

Boundary conditions: opposite displacement (left and right) along the x direction.

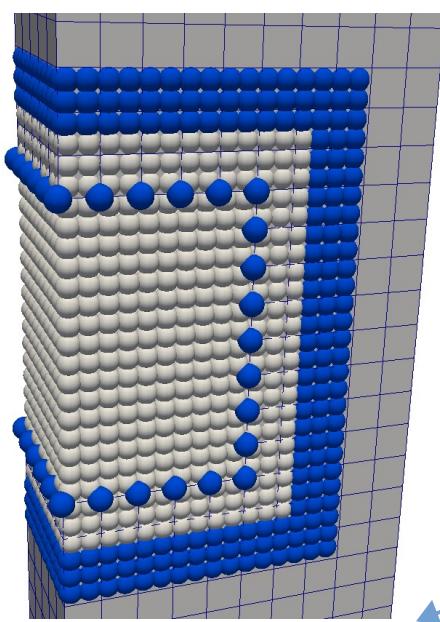


CRACK TEST

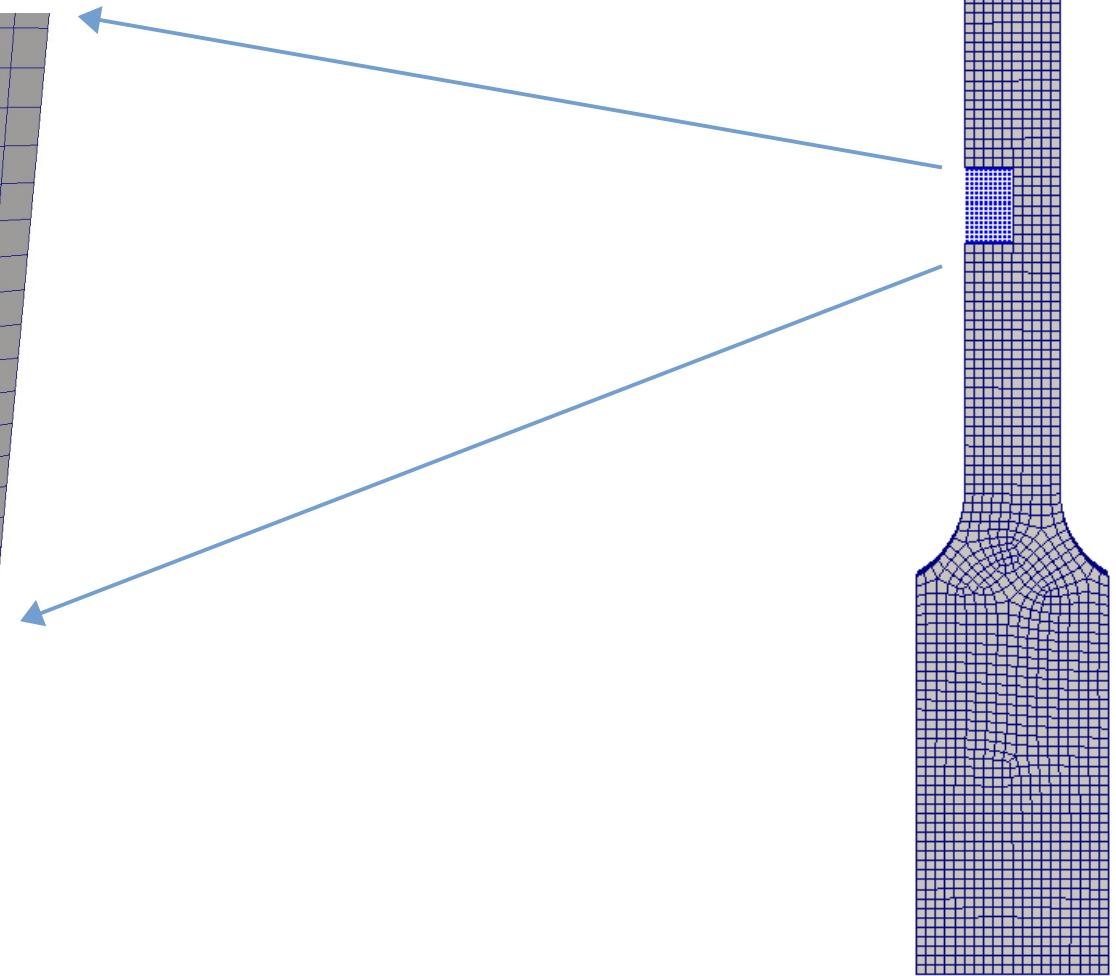
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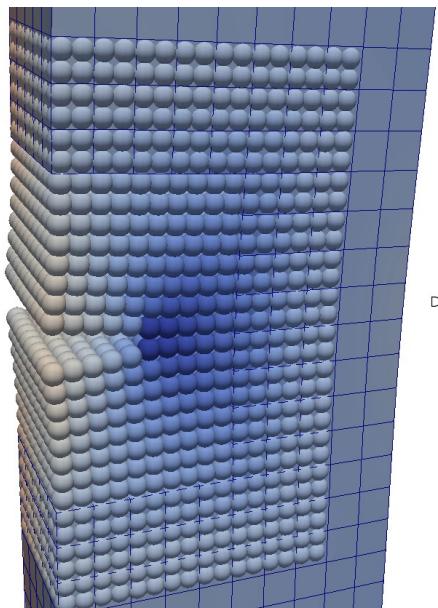
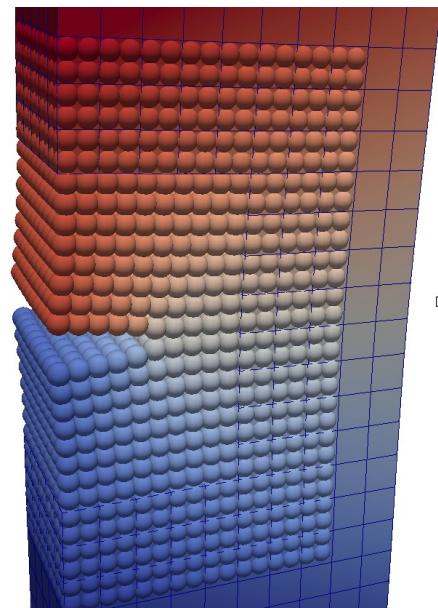
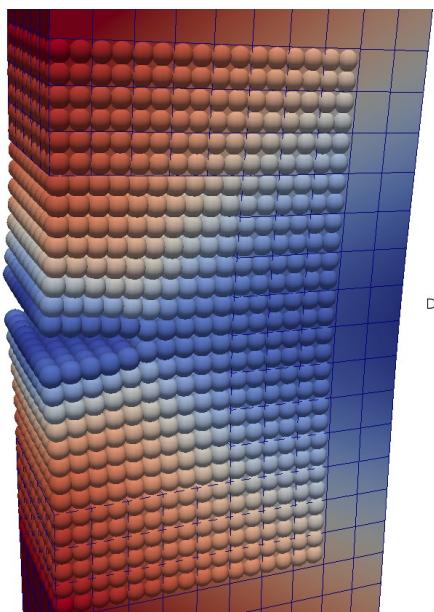
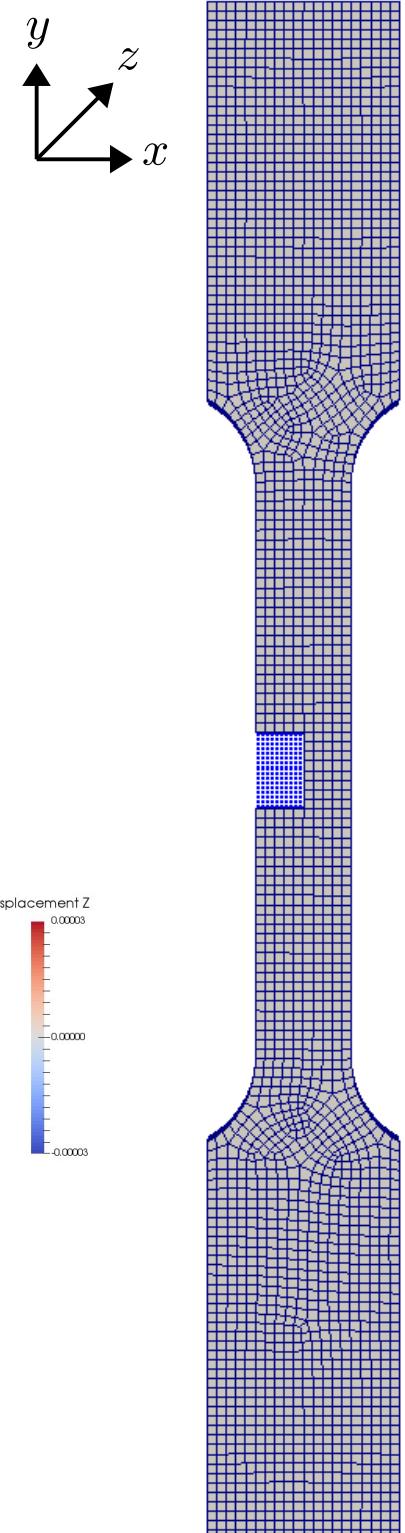
TENSILE BAR



control nodes



TENSILE BAR – WITH CRACK



ANOTHER CRACK TEST

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

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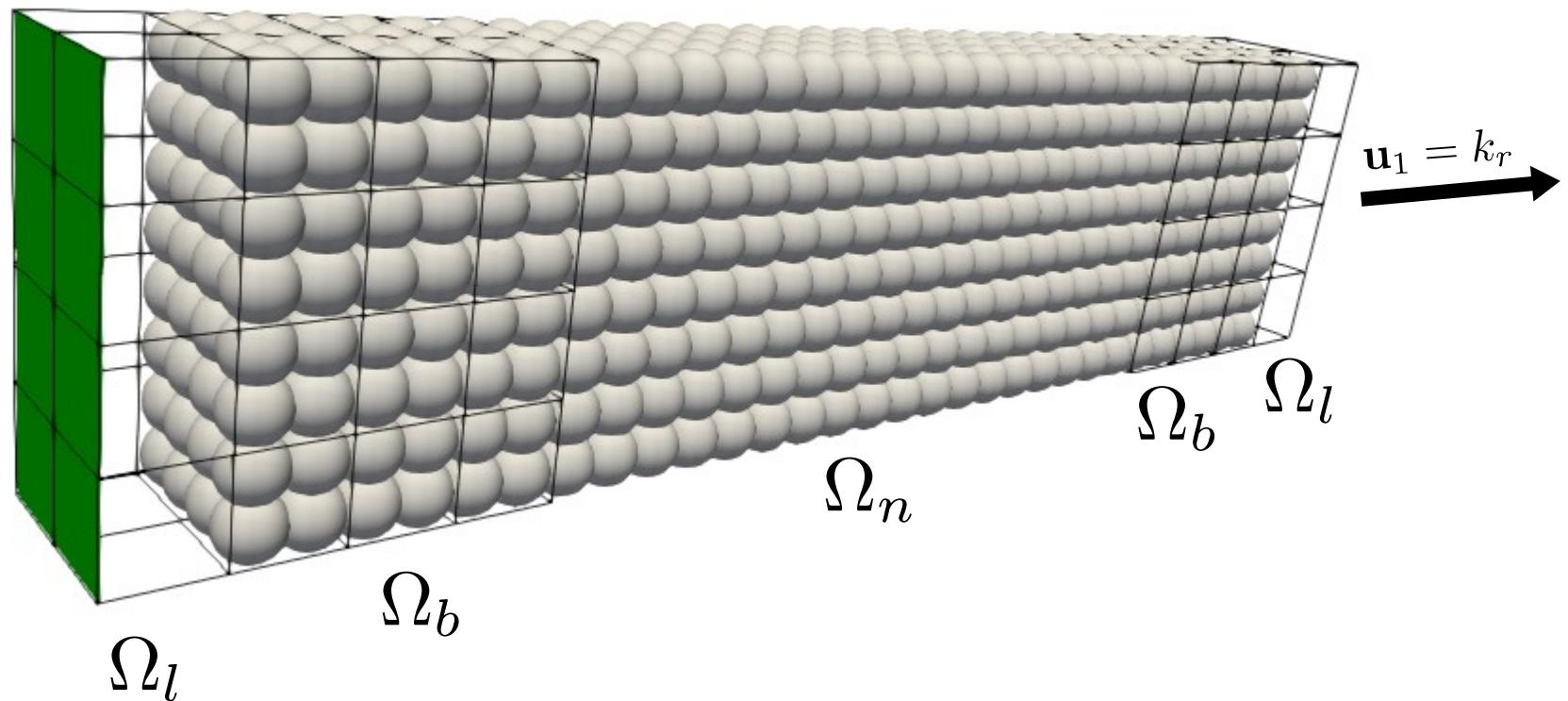
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Neumann:

$$p = -\bar{p}$$

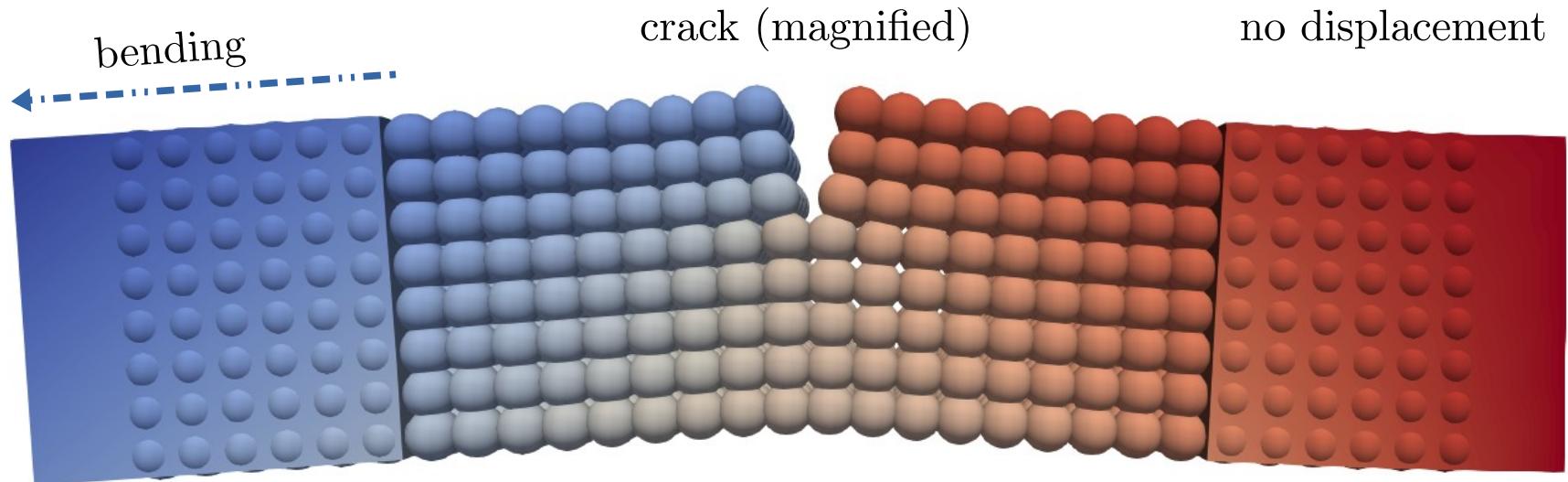


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- developing a **unified theory** for nonlocal operators (more soon...)
- **unifying** the fractional and nonlocal communities (more in December)

MANNA Modeling, Analysis and Numerics for Nonlocal Applications, Santa Fe, NM, Dec. 11–15, 2017

Co-Organizers

M. D'Elia

G. E. Karniadakis

Scientific Committee

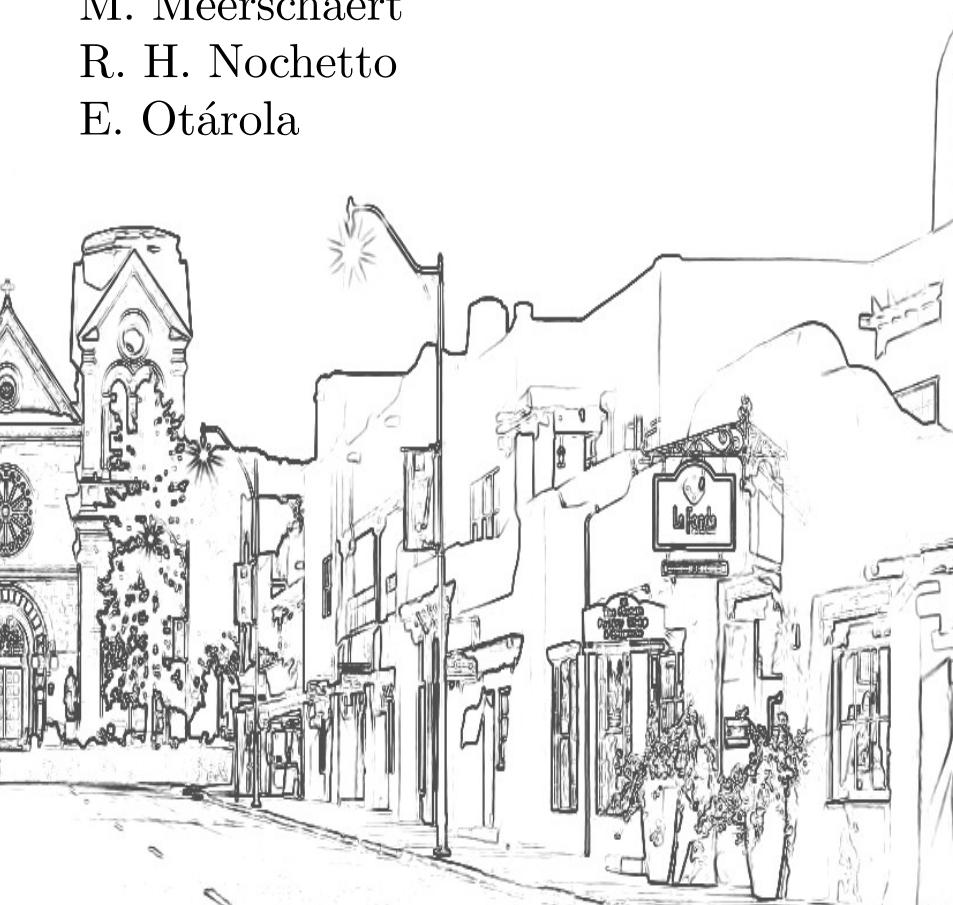
Q. Du

M. Gunzburger

M. Meerschaert

R. H. Nochetto

E. Otárola



Course lecturers

D. del Castillo Negrete

D. Littlewood

F. Mainardi

A. Salgado

P. Seleson

M. Zayernouri

Workshop speakers

B. Alali

P. Bochev

A. Bonito

K. Burrage

W. Deng

K. Diethelm

V. Ervin

R. Garrappa

R. Lehoucq

R. Lipton

R. Metzler

G. McKinley

E. Nan

P. Radu

M. Stynes

S. Silling

A. Sikorskii

H. Wang

Y. Zhang

Thank you