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A coupling strategy for Local and Nonlocal continuum models

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

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INTRODUCTION

NONLOCAL MODELS

nonlocal models are used in several diverse applications

our interest: nonlocal diffusion operators

- peridynamic model for mechanics
- jump processes
- nonlocal heat conduction
- image analyses
- machine learning

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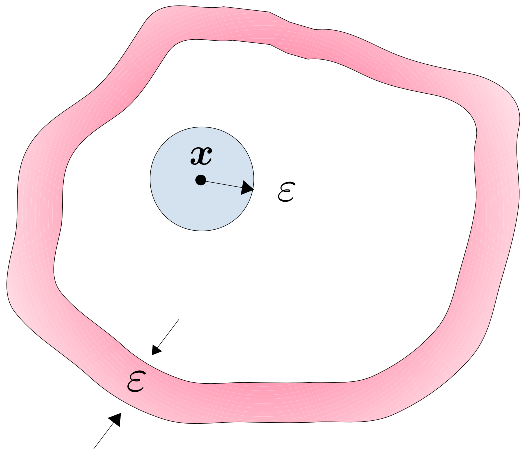
how do they look like?

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

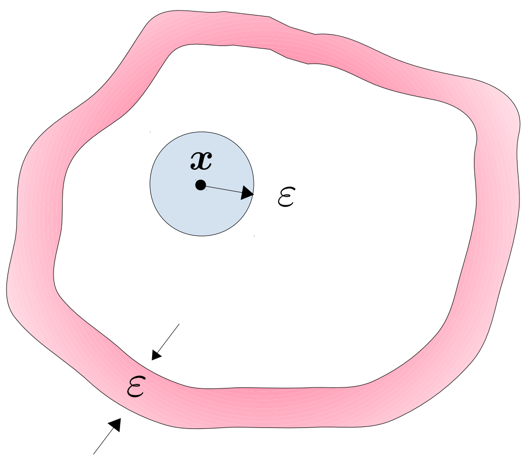
NONLOCAL MODELS

- interactions can occur at distance, without contact
- used in many scientific and engineering applications, where the material dynamics depends on microstructure



NONLOCAL MODELS

- 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**[1] and physics-based **nonlocal elasticity**[2] which can model fractures and material failures
- nonlocal models are required to accurately resolve **small scale features**, e.g. crack tips or dislocations



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:

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

- we have **well–posedness** results for a large class of nonlocal steady and unsteady–state equations, control problems and parameter identification

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

NONLOCAL vs LOCAL

facts:

- the numerical solution of nonlocal models might be prohibitively expensive
- we can compute the solution of PDEs efficiently

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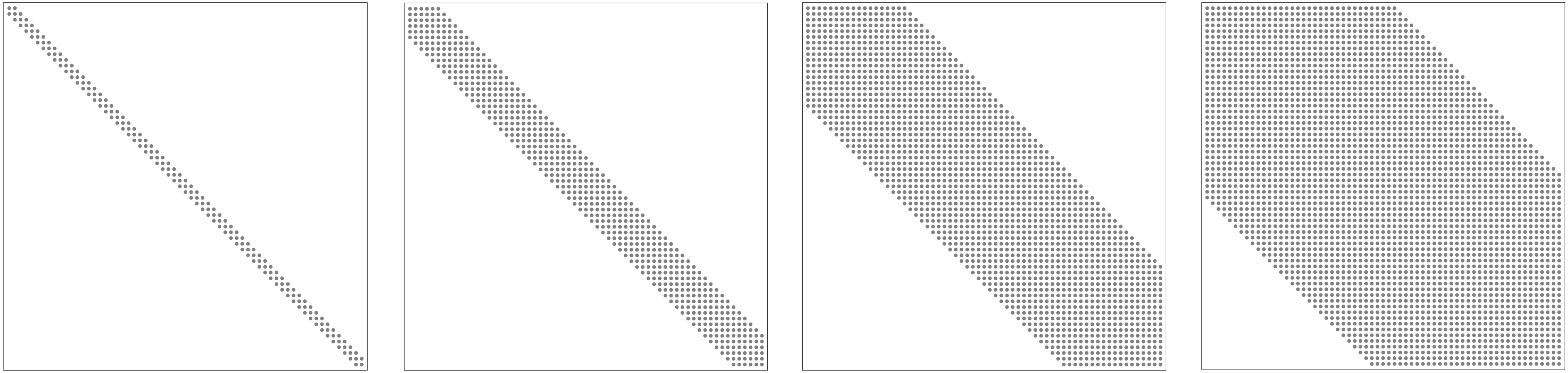
• we can compute the solution of PDEs efficiently

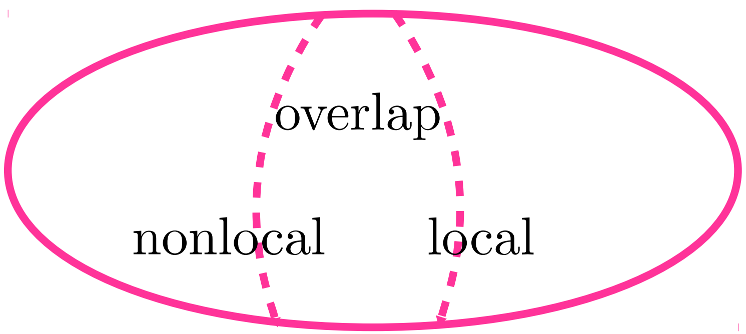


→ increasing interaction radius →

WHAT ABOUT COUPLING?

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

• split the computational domain in a local and a nonlocal domain and **couple**, in a smart way, the models at the interfaces or overlapping regions



WHAT ABOUT COUPLING?

Contribution: define and analyze a local-to-nonlocal **(LtN)** coupling method for nonlocal diffusion models that

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

WHAT ABOUT COUPLING?

Contribution: define and analyze a local-to-nonlocal **(LtN)** coupling method for nonlocal diffusion models that

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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

- Notation
- Formulation of the optimization problem
- Finite dimensional approximation
- Numerical tests

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
- allows us to study nonlocal diffusion similarly to the classical, local, counterpart

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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: $\mathcal{L}u(\boldsymbol{x}) = \mathcal{D}(\boldsymbol{\Phi}\mathcal{G}u(\boldsymbol{x}))$

$$\mathcal{L}u(\boldsymbol{x}) = 2\int_{\mathbb{R}^n} \big(u(\boldsymbol{y}) - u(\boldsymbol{x})\big)\, \underline{\boldsymbol{\alpha}(\boldsymbol{x},\boldsymbol{y}) \cdot \big(\boldsymbol{\Phi}(\boldsymbol{x},\boldsymbol{y})\boldsymbol{\alpha}(\boldsymbol{x},\boldsymbol{y})}\big)\, d\boldsymbol{y}$$

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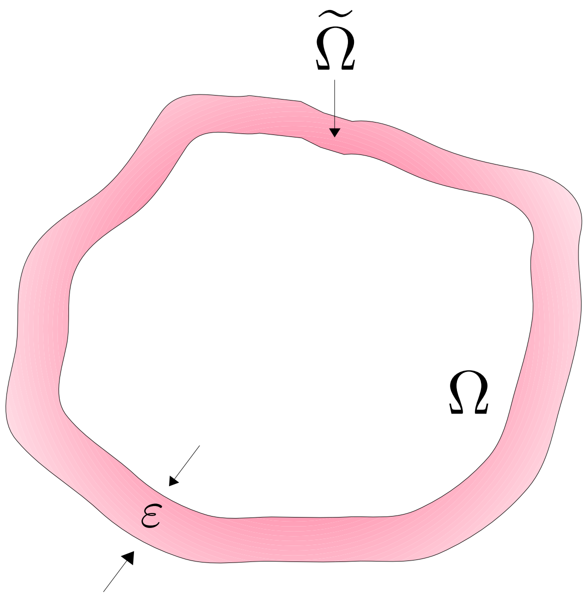
$$\mathcal{L}u(\boldsymbol{x}) = 2\int_{\mathbb{R}^n} \big(u(\boldsymbol{y}) - u(\boldsymbol{x})\big)\, \gamma(\boldsymbol{x},\boldsymbol{y})\, d\boldsymbol{y}$$

NONLOCAL VECTOR CALCULUS

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

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

Define: $\Omega^+ = \Omega \cup \widetilde{\Omega}$



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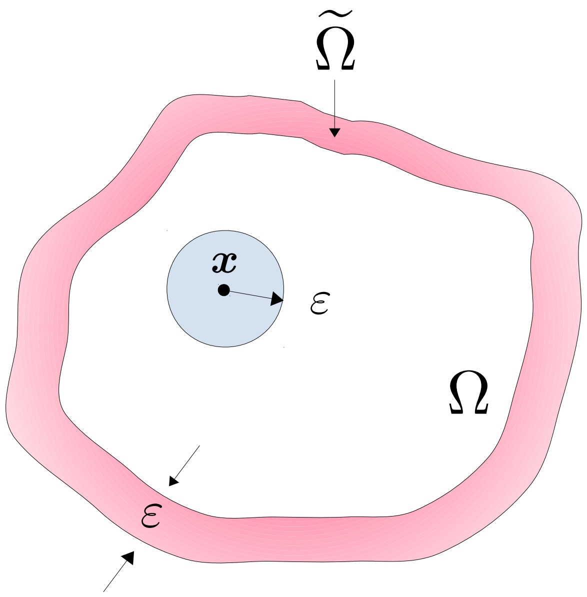


Kernel: we assume

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

$$B_\varepsilon(\boldsymbol{x}) = \{\boldsymbol{y} \in \Omega^+ : \ |\boldsymbol{x} - \boldsymbol{y}| < \varepsilon, \ \boldsymbol{x} \in \Omega\}$$

THE LtN 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, *submitted*, 2015

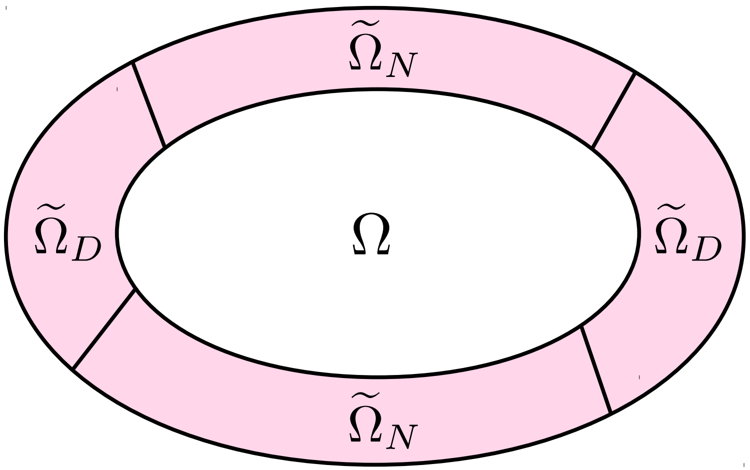
MODEL PROBLEMS

The nonlocal problem

$$\begin{cases} -\mathcal{L}u_n = f_n & \boldsymbol{x} \in \Omega \\ u_n = \sigma_n & \boldsymbol{x} \in \widetilde{\Omega}_D \\ -\mathcal{N}(\mathcal{G}u_n) = \eta_n & \boldsymbol{x} \in \widetilde{\Omega}_N, \end{cases}$$

where $\sigma_n \in \widetilde{V}(\widetilde{\Omega})$, $f_n \in L^2(\Omega)$ and $\eta_n \in L^2(\widetilde{\Omega}_N)$

nonlocal counterpart of a Neumann condition



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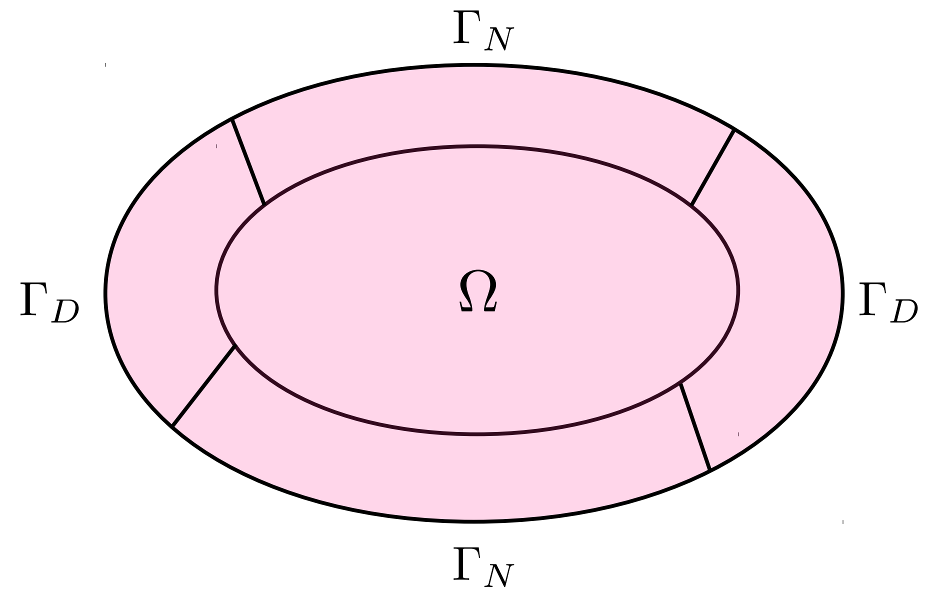
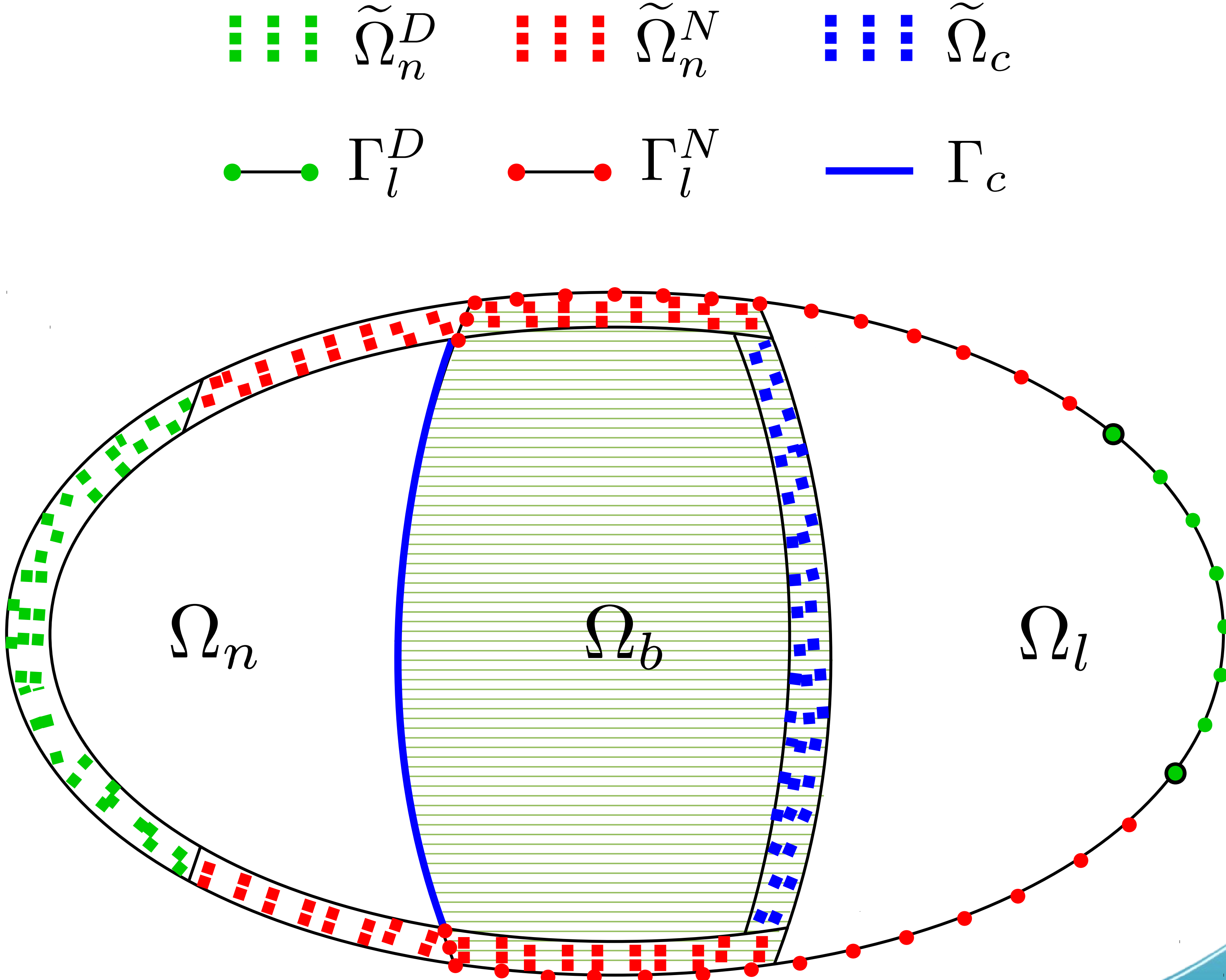


The local problem (Poisson equation)

$$\begin{cases} -\Delta u_l = f_l & \boldsymbol{x} \in \Omega^+ \\ u_l = \sigma_l & \boldsymbol{x} \in \Gamma_D \\ \nabla u_l \cdot \mathbf{n} = \eta_l & \boldsymbol{x} \in \Gamma_N, \end{cases}$$

where $f_l \in L^2(\Omega)$, $\sigma_l \in H^{\frac{1}{2}}(\Gamma_D)$ and $\eta_l \in L^2(\Gamma_N)$

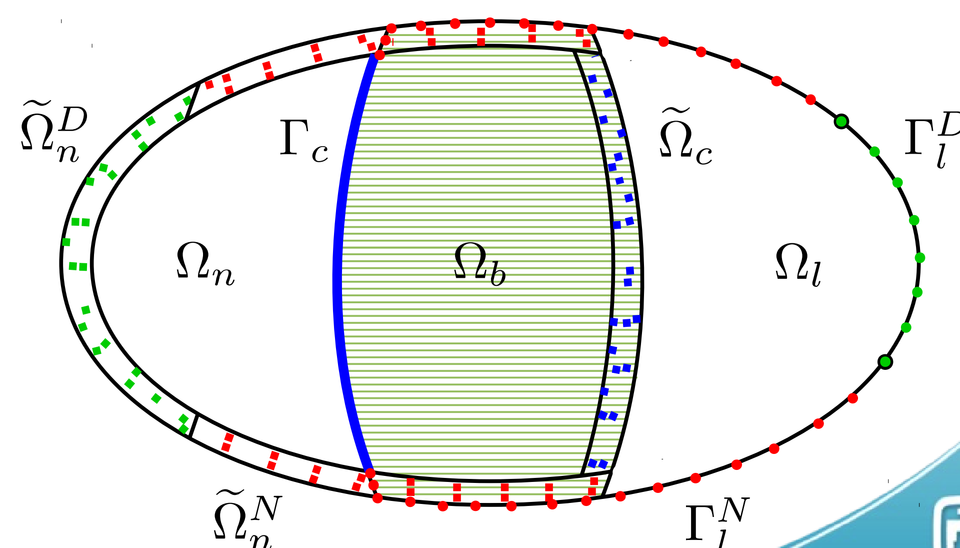
LtN COUPLING



LtN COUPLING

State equations:

$$\begin{cases} -\mathcal{L}u_n = f_n & \boldsymbol{x} \in \Omega_n \\ u_n = \theta_n & \boldsymbol{x} \in \widetilde{\Omega}_c \\ u_n = 0 & \boldsymbol{x} \in \Omega_n^D \\ -\mathcal{N}(\mathcal{G}u_n) = 0 & \boldsymbol{x} \in \widetilde{\Omega}_n^N \end{cases} \quad \text{and} \quad \begin{cases} -\Delta u_l = f_l & \boldsymbol{x} \in \Omega_l \\ u_l = \theta_l & \boldsymbol{x} \in \Gamma_c \\ u_l = 0 & \boldsymbol{x} \in \Gamma_l^D \\ \nabla u_l \cdot \mathbf{n} = 0 & \boldsymbol{x} \in \Gamma_l^N, \end{cases}$$

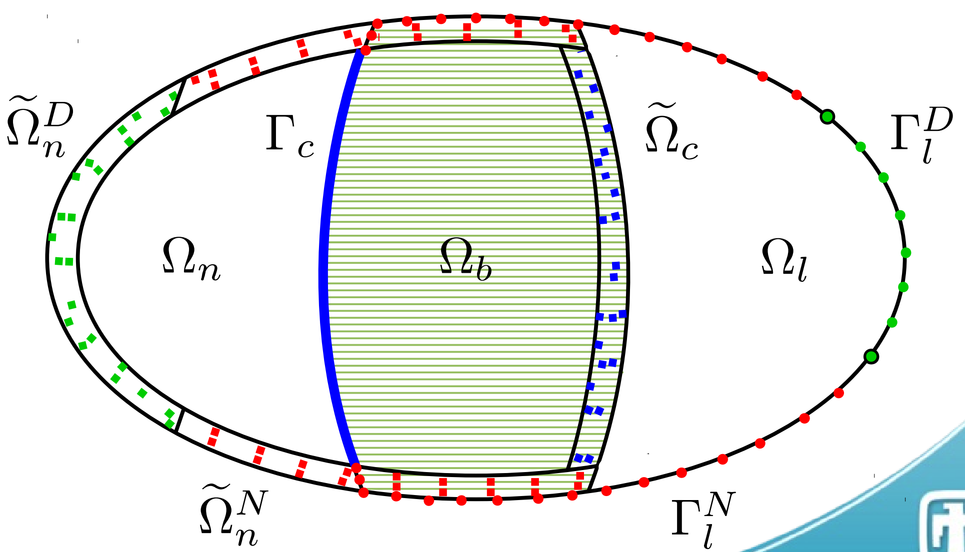


LtN COUPLING

Optimization problem:

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

$$\text{s.t.}\left\{\begin{array}{rcll} -\mathcal{L}u_n &=& f_n & \boldsymbol{x}\in\Omega_n\\ u_n &=& \theta_n & \boldsymbol{x}\in\widetilde{\Omega}_c\\ u_n &=& 0 & \boldsymbol{x}\in\Omega_n^D\\ -\mathcal{N}(\mathcal{G}u_n) &=& 0 & \boldsymbol{x}\in\widetilde{\Omega}_n^N \end{array}\right. \quad\text{and}\quad \left\{\begin{array}{rcll} -\Delta u_l &=& f_l & \boldsymbol{x}\in\Omega_l\\ u_l &=& \theta_l & \boldsymbol{x}\in\Gamma_c\\ u_l &=& 0 & \boldsymbol{x}\in\Gamma_l^D\\ \nabla u_l\cdot\mathbf{n} &=& 0 & \boldsymbol{x}\in\Gamma_l^N, \end{array}\right.$$



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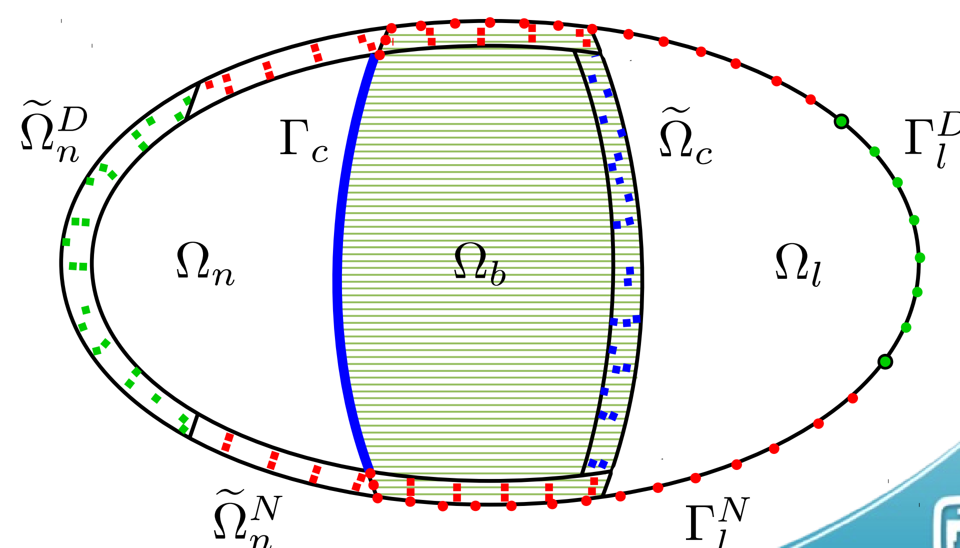
control variables $(\theta_n,\theta_l)\in\Theta_n\times\Theta_l = \{(\sigma_n,\sigma_l):\sigma_n\in\widetilde{V}_{\widetilde{\Omega}_i}(\widetilde{\Omega}_c),\ \sigma_l\in H^{\frac{1}{2}}(\Gamma_c)\}$



LtN COUPLING

LtN solution

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

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

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Questions:

- is it unique?
- what is the "error" wrt the global nonlocal solution $\widehat{u}_n$?

$$\begin{cases} -\mathcal{L}\widehat{u}_n & = & f & \boldsymbol{x} \in \Omega \\ \widehat{u}_n & = & 0 & \boldsymbol{x} \in \widetilde{\Omega}_D \\ -\mathcal{N}(\mathcal{G}u_n) & = & 0 & \boldsymbol{x} \in \widetilde{\Omega}_N \end{cases}$$

IS THE SOLUTION UNIQUE?

Reduced form:

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

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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

$$\left\{\begin{array}{rll} -\mathcal{L}v_n & = 0 & \boldsymbol{x}\in\Omega_n \\ v_n & = \theta_n & \boldsymbol{x}\in\widetilde{\Omega}_c \\ +\,\mathrm{VC} & & \end{array}\right. \qquad \text{and} \qquad \left\{\begin{array}{rll} -\Delta v_l & = 0 & \boldsymbol{x}\in\Omega_l \\ v_l & = \theta_l & \boldsymbol{x}\in\Gamma_c \\ +\,\mathrm{BC} & & \end{array}\right.$$

homogeneous components u_n^0 and u_l^0

$$\left\{\begin{array}{rll} -\mathcal{L}u_n^0 & = f_n & \boldsymbol{x}\in\Omega_n \\ v_n & = 0 & \boldsymbol{x}\in\widetilde{\Omega}_c \\ +\,\mathrm{VC} & & \end{array}\right. \qquad \text{and} \qquad \left\{\begin{array}{rll} -\Delta u_l^0 & = f_l & \boldsymbol{x}\in\Omega_l \\ v_l & = 0 & \boldsymbol{x}\in\Gamma_c \\ +\,\mathrm{BC} & & \end{array}\right.$$

IS THE SOLUTION UNIQUE?

Reduced functional:

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

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

IS THE SOLUTION UNIQUE?

Reduced functional:

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

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

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

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

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

defines a norm in the control variable space

ASSUMPTIONS, LEMMAS AND TOOLS

Assumptions:

- $\overline{\gamma}_k = \|\gamma_k\|_\infty^{1/k} < \infty \quad$ with $\quad \gamma_k(\boldsymbol{x}) = \int_{\Omega^+} \gamma^k(\boldsymbol{x}, \boldsymbol{y})\, d\boldsymbol{y}, \quad k = 1, 2$

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Lemmas:

- nonlocal trace inequality
- nonlocal maximum principle
- strong Cauchy-Schwarz inequality for the harmonic components

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

Tools:

- nonlocal vector calculus

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, *submitted*, 2015

THE DISCRETIZATION

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

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

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strong form + particle method — **weak form + finite element method**

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strong form + particle method   **weak form + finite element method**

Advantage: the particle and finite element solvers can be used as **black boxes**

THE DISCRETIZATION

Note: the nonlocal solution is defined on points while the local solution is a piecewise polynomial over the computational domain

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A modified functional: pointwise misfit

$$J_d(\mathbf{u}_n, \mathbf{u}_l) = \frac{1}{2}\sum_{i=1}^{n_b}\big((S_n\mathbf{u}_n)_i - (S_l\mathbf{u}_l)_i\big)^2 = \frac{1}{2}\|S_n\mathbf{u}_n - S_l\mathbf{u}_l\|_2^2.$$

S_n: nonlocal **selection matrix**

S_l: $(S_l)_{ij} = \phi_j(x_i)$, where ϕ_j is the j-th FE basis

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What about uniqueness?

THE ALGORITHM

A gradient–based algorithm

Given an initial guess $\theta^0_{nh}, \theta^0_{lh}$, for $k = 0, 1, 2, \ldots$

1. **solve the state** equations to obtain $u^k_{nh}(\theta^k_{nh})$ and $u^k_{lh}(\theta^k_{nh})$ and compute J_h
2. **compute the gradient** of the functional and evaluate it $\left.\dfrac{\mathrm{d}J_h}{\mathrm{d}(\theta_{nh}, \theta_{lh})}\right|_{(\theta^k_{nh}, \theta^k_{lh})}$
3. Use 1. and 2. to **compute the increments** $\delta(\theta^k_{nh})$ and $\delta(\theta^k_{lh})$
4. Set $\theta^{k+1}_{nh} = \theta^k_{nh} + \delta(\theta^k_{nh})$, and $\theta^{k+1}_{lh} = \theta^k_{lh} + \delta(\theta^k_{lh})$

THE ALGORITHM

A gradient–based algorithm

Given an initial guess $\theta^0_{nh}, \theta^0_{lh}$, for $k = 0, 1, 2, \ldots$

1. **solve the state** equations to obtain $u^k_{nh}(\theta^k_{nh})$ and $u^k_{lh}(\theta^k_{nh})$ and compute J_h
2. **compute the gradient** of the functional and evaluate it $\left.\dfrac{\mathrm{d}J_h}{\mathrm{d}(\theta_{nh}, \theta_{lh})}\right|_{(\theta^k_{nh}, \theta^k_{lh})}$
3. Use 1. and 2. to **compute the increments** $\delta(\theta^k_{nh})$ and $\delta(\theta^k_{lh})$ $\rightarrow$ **BFGS algorithm**
4. Set $\theta^{k+1}_{nh} = \theta^k_{nh} + \delta(\theta^k_{nh})$, and $\theta^{k+1}_{lh} = \theta^k_{lh} + \delta(\theta^k_{lh})$

NUMERICAL TESTS

– 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, *submitted*, 2015

GEOMETRY

Coupling Peridigm and Albany

peridigm.sandia.gov

software.sandia.gov/albany/

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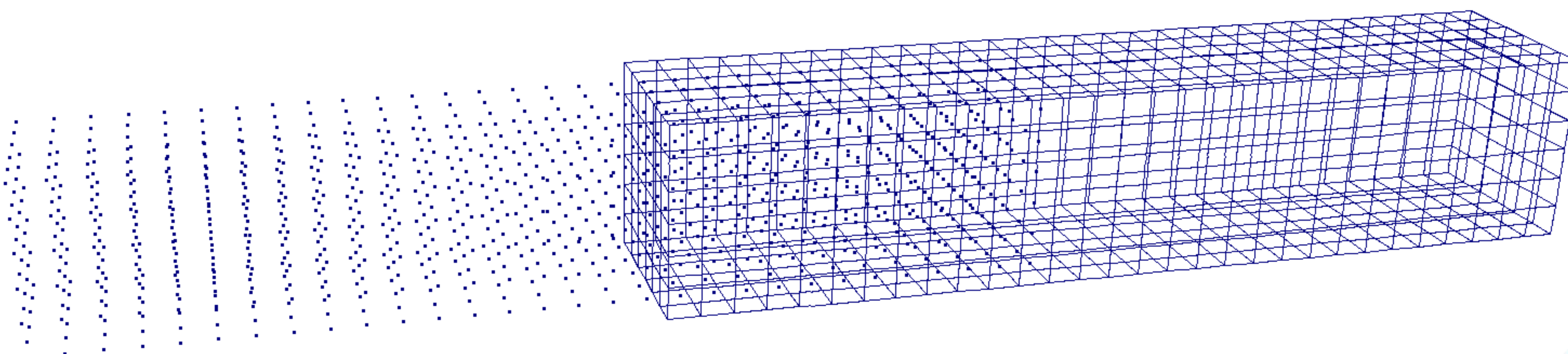


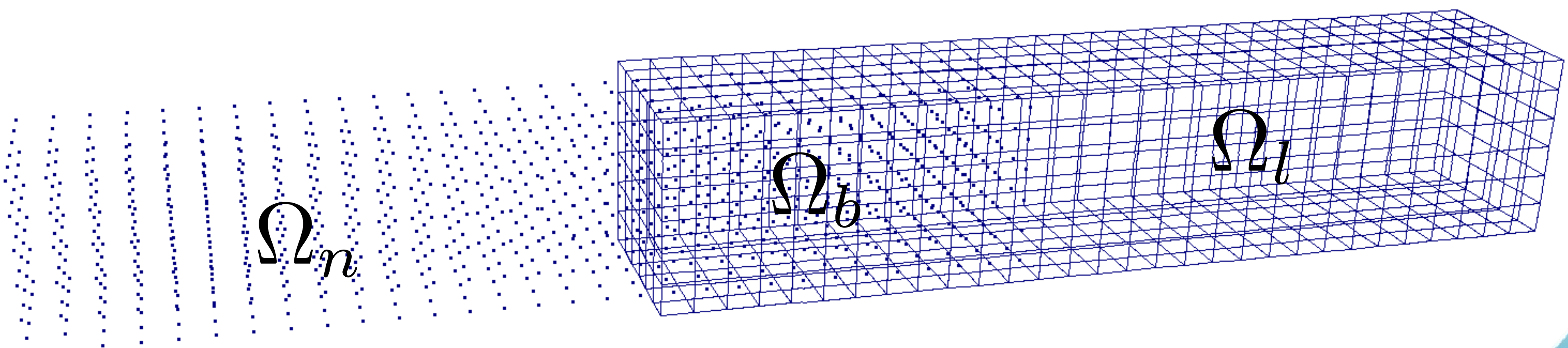
GEOMETRY

Nonlocal domain: $\Omega_n := [0,\ 2.5] \times [0,\ 0.5] \times [0,\ 0.5]$

Local domain: $\Omega_l := [1.5,\ 4] \times [0,\ 0.5] \times [0,\ 0.5]$

Overlap domain: $\Omega_b := [1.5,\ 2.5] \times [0,\ 0.5] \times [0,\ 0.5]$

Kernel: $$\gamma(\boldsymbol{x}, \boldsymbol{y}) = \begin{cases} \dfrac{3}{\pi\varepsilon^4} \dfrac{1}{\|\boldsymbol{x}-\boldsymbol{y}\|} & \|\boldsymbol{x}-\boldsymbol{y}\| \le \varepsilon \\ 0 & \text{otherwise,} \end{cases}$$



THE PATCH TEST

Analytic solution: $u^*_{anl} = x - \frac{5}{3}$, prescribed in $0 \le x \le 0.5$ and on $x = 4$

LtN control: initialized at zero in $2 \le x \le 2.5$ and on $x = 1.5$

THE PATCH TEST

Analytic solution: $u^*_{anl} = x - \dfrac{5}{3}$, prescribed in $0 \leq x \leq 0.5$ and on $x = 4$

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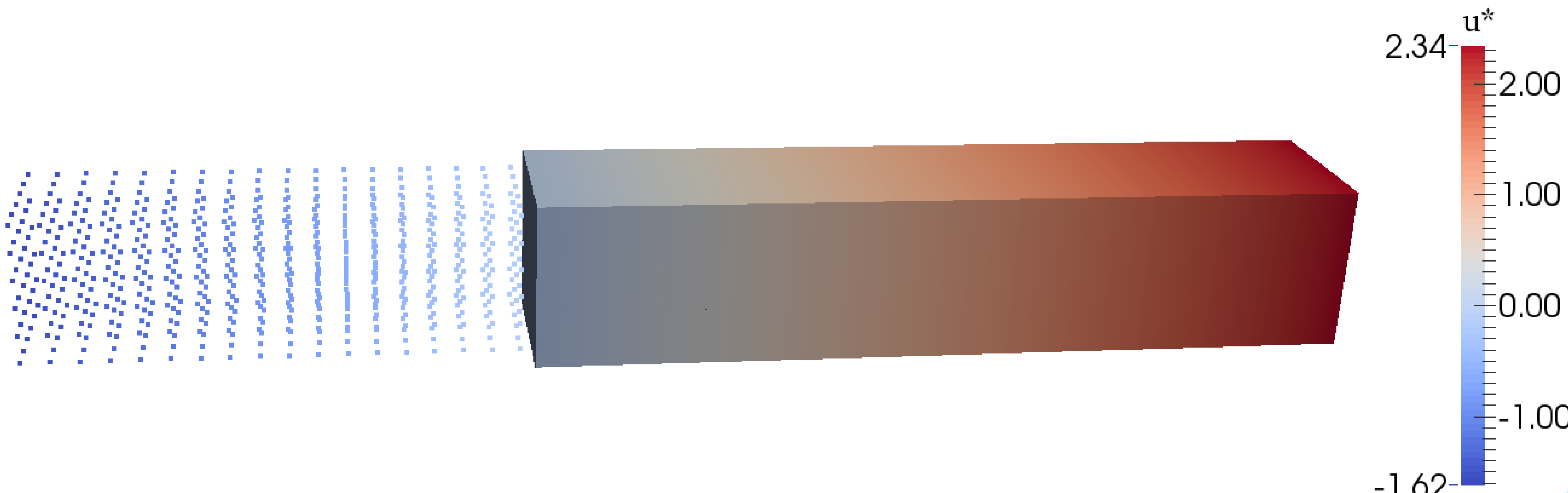
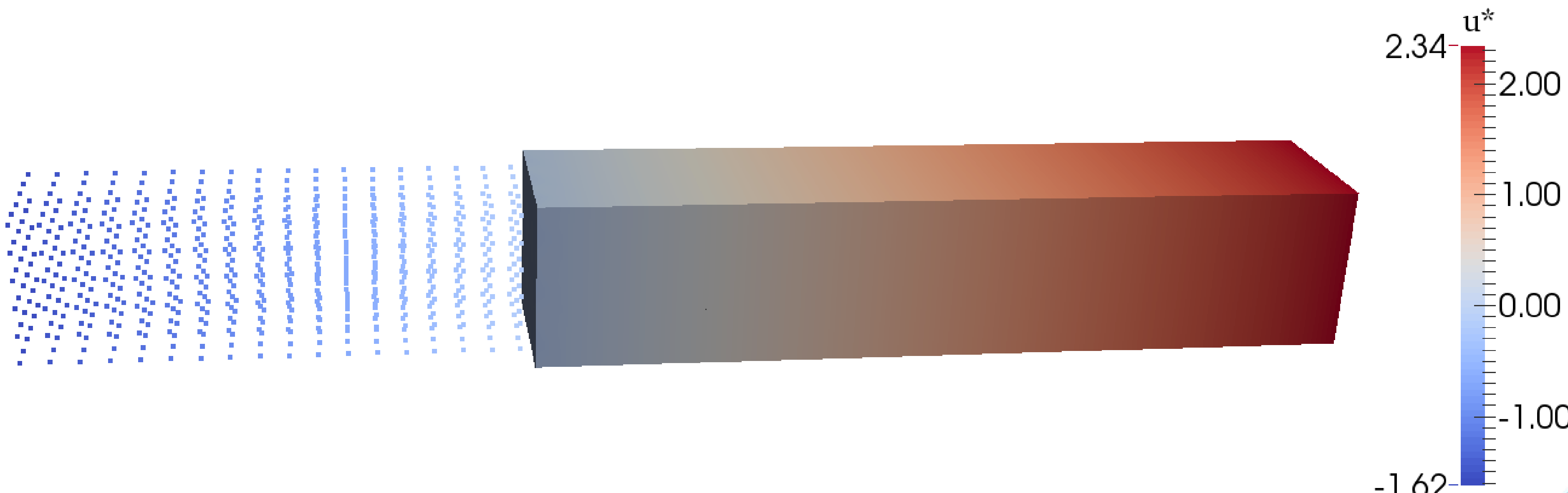


THE PATCH TEST

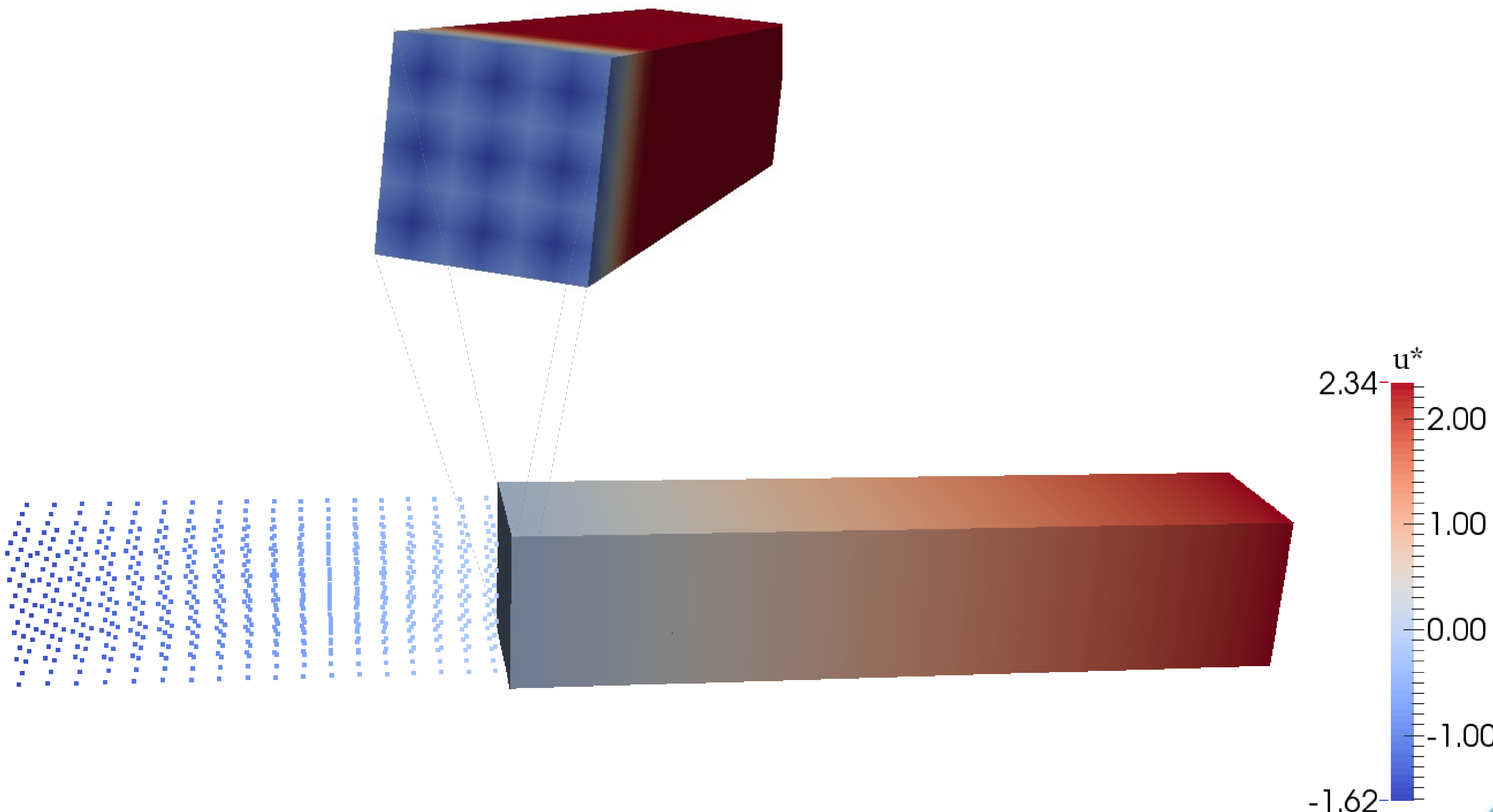
Analytic solution: $u^*_{anl} = x - \dfrac{5}{3}$, prescribed in $0 \leq x \leq 0.5$ and on $x = 4$

LtN control: initialized at zero in $2 \leq x \leq 2.5$ and on $x = 1.5$



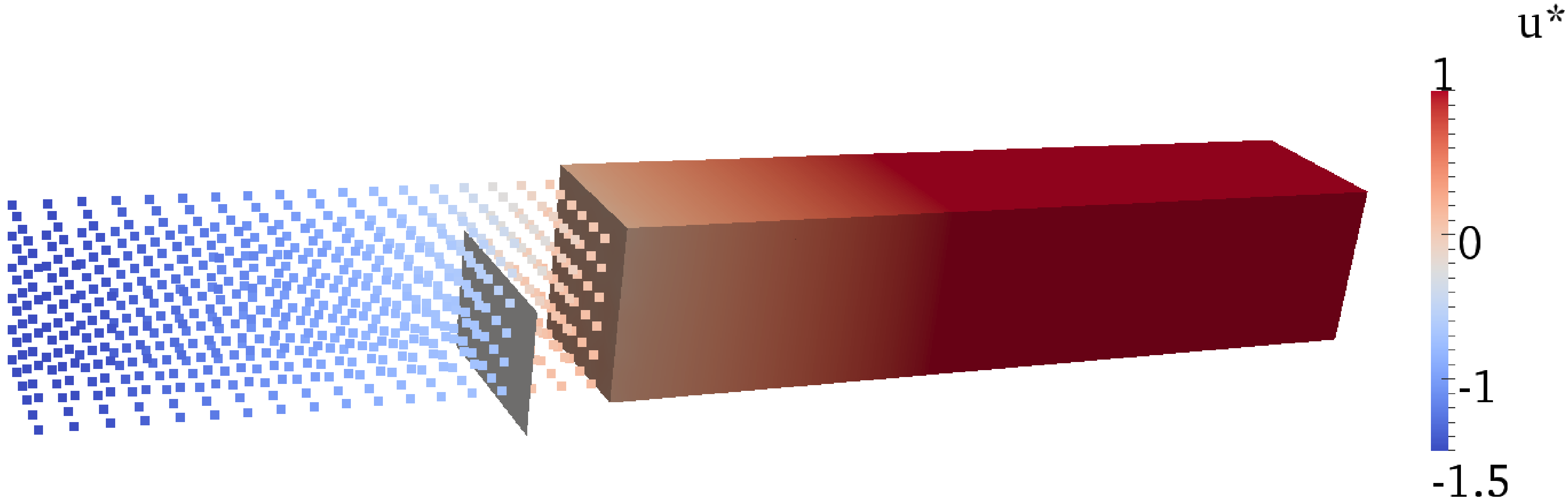
What about uniqueness?

THE PATCH TEST

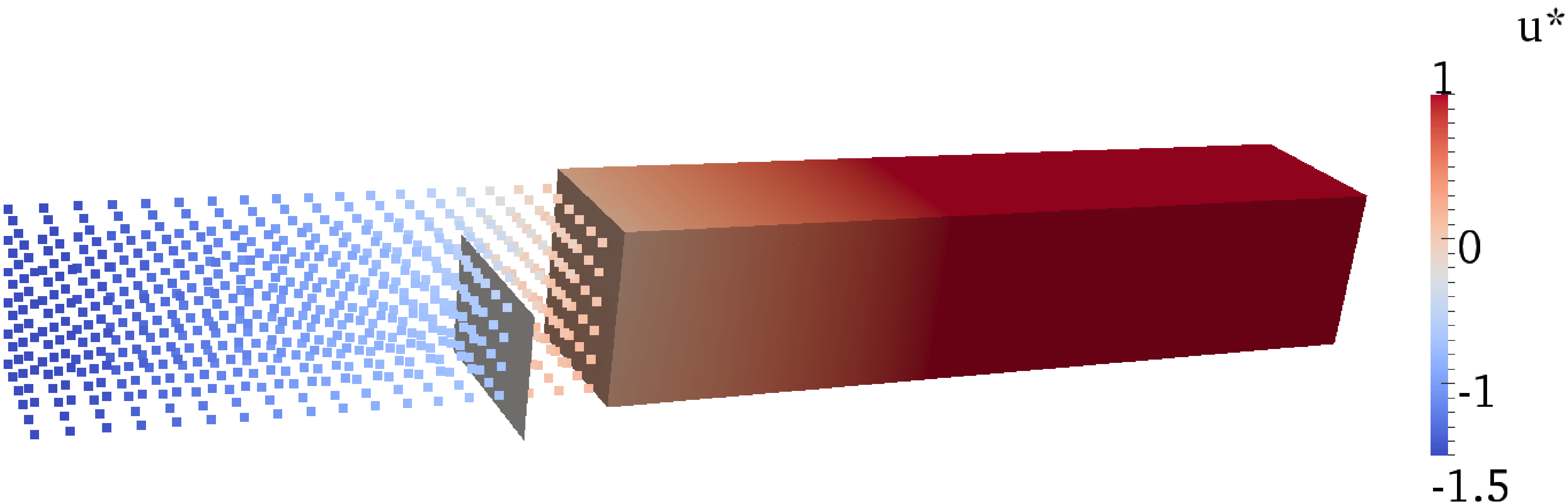


What about uniqueness?

MANAGING A CRACK



MANAGING A CRACK



Lots of things to do!

- time dependent problems
- crack propagation
- real geometries
- improve performance
- better initialization

Thank you