

Formulation and Analysis of an SAND2015-4820C **Optimization-Based Local to Nonlocal** coupling method

Marta D'Elia, joint work with **Pavel Bochev**

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June 22nd 2015, **GRAZ**

From Open to Closed Loop Control

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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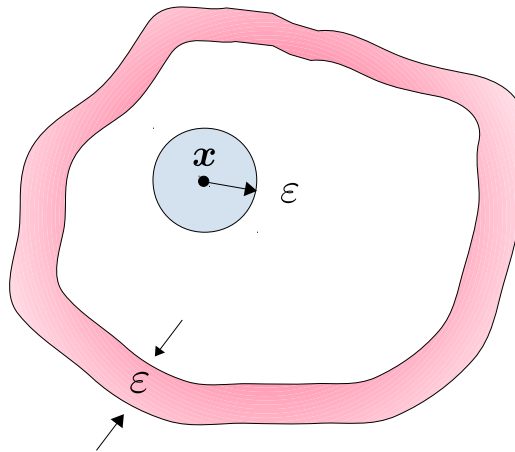
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how do they look like?

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

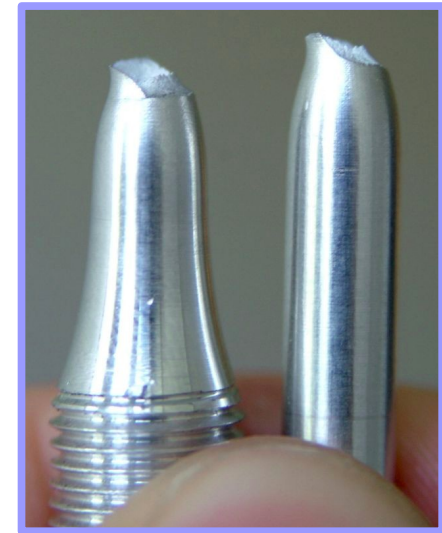
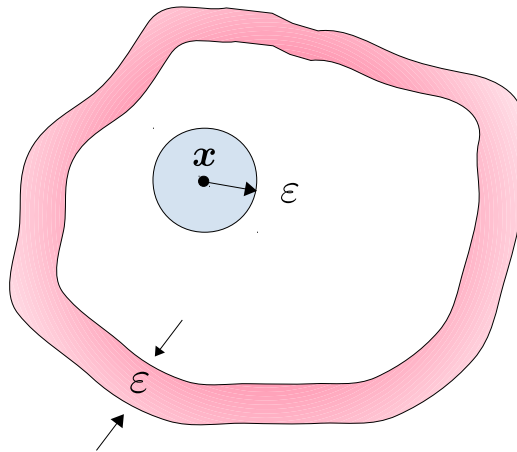
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- used in many scientific and engineering applications, where the material dynamics depends on microstructure
- example: nonlocal continuum mechanics theories, e.g. [peridynamics](#)[1] and physics-based [nonlocal elasticity](#)[2] which can model fractures and material failures
- nonlocal models are required to accurately resolve [small scale features](#), e.g. crack tips or dislocations

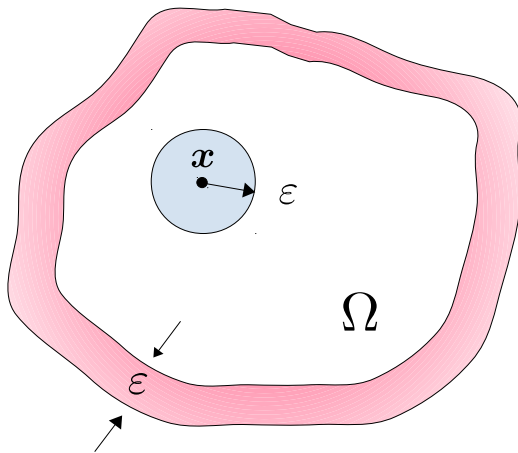


- [1] S.Silling, R.B.Lehoucq, Advances in Applied Mechanics, Elsevier, 2010.
[2] M.Di Paola, G.Failla, and M.Zingales, Journal of Elasticity, 2009.

ductile fracture,
Wikipedia

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- **example:** estimate the first exit time of a particle from a bounded domain [3]



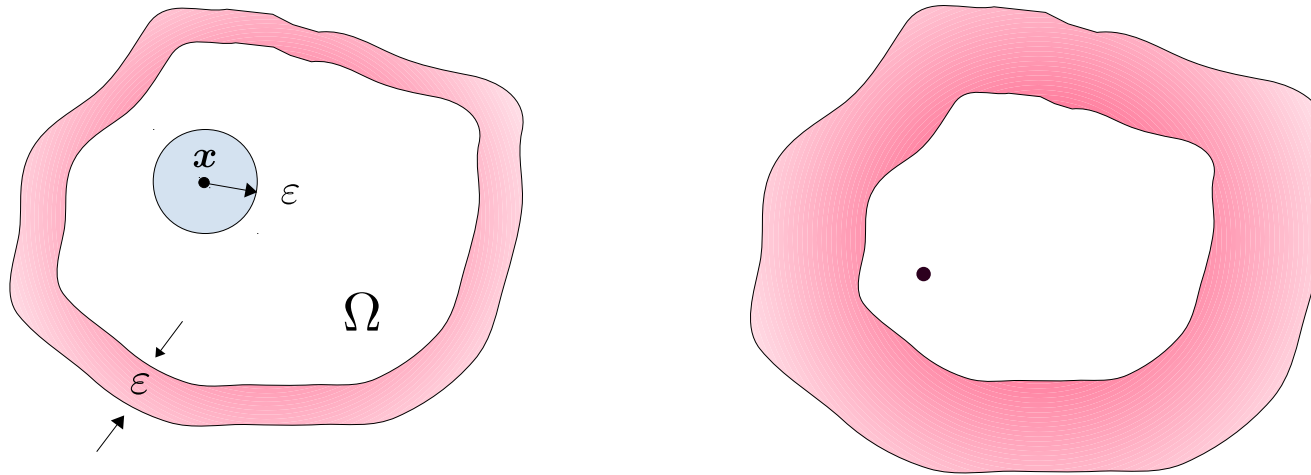
[1] M. D'Elia, Q. Du, M. Gunzburger, R. Lehoucq, submitted, 2014

[2] O. Defterli, M. D'Elia, Q. Du, M. Gunzburger, R. Lehoucq, M.M. Meerschaert, Fractional Derivatives and Applications, 2015

[3] N. Burch, M. D'Elia, R. Lehoucq, The European Physical Journal Special Topics, 2014

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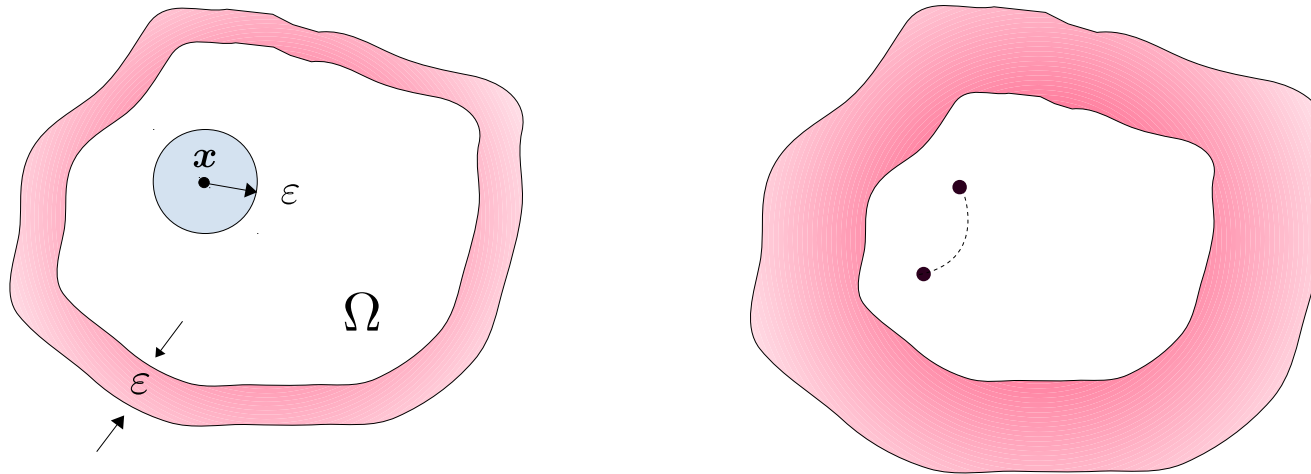
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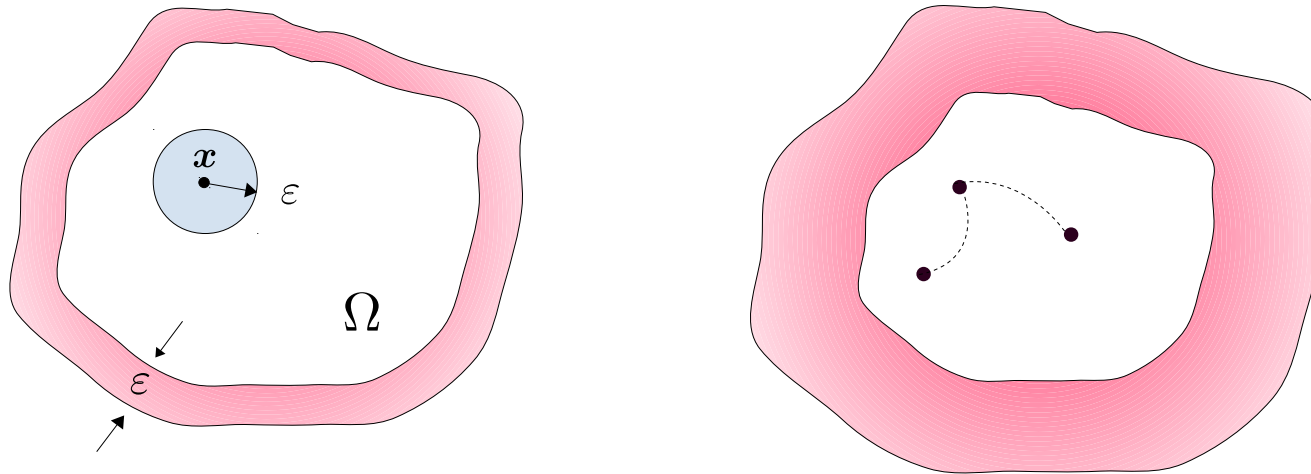
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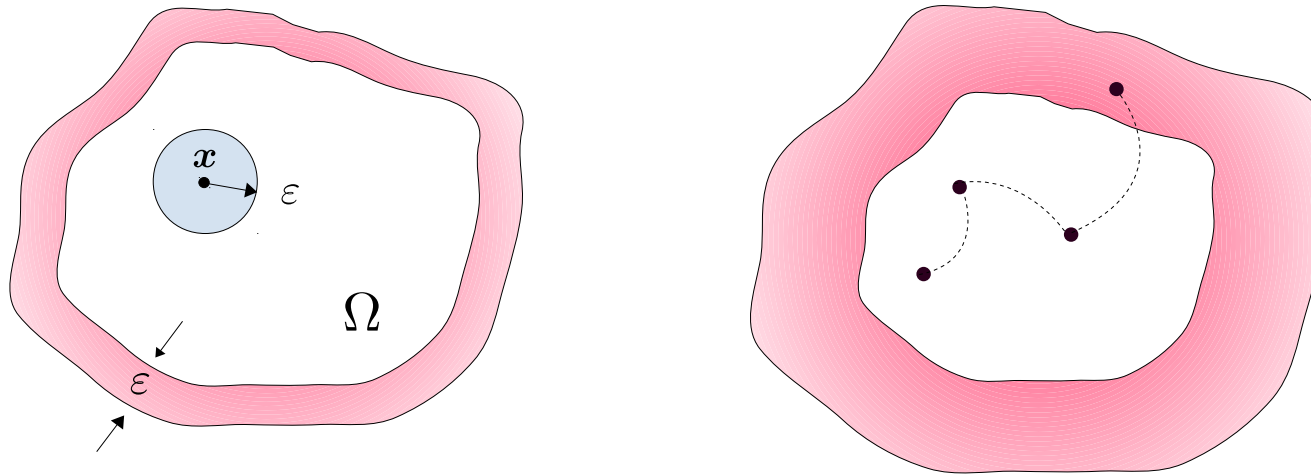
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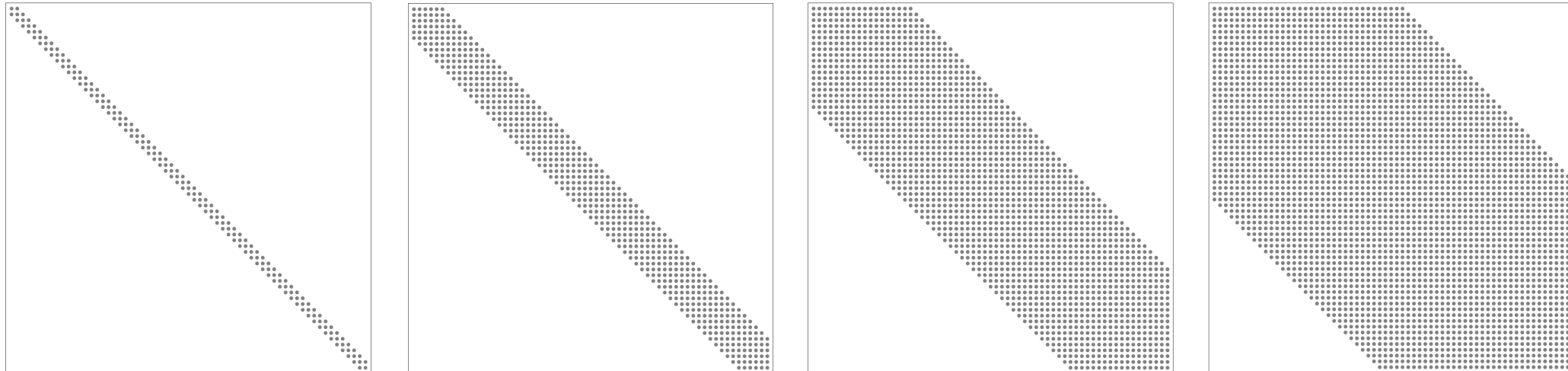
- facts:**
- a recently developed theoretical and numerical analysis allows us to study nonlocal problems **similarly** to the local (classical) counterpart
 - we have **well-posedness** results for a large class of nonlocal steady and unsteady-state equations
 - we have **numerical convergence** results 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

NONLOCAL vs LOCAL

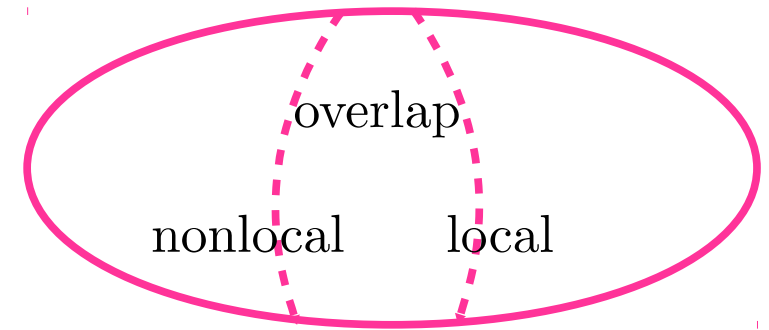
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→ increasing interaction radius →

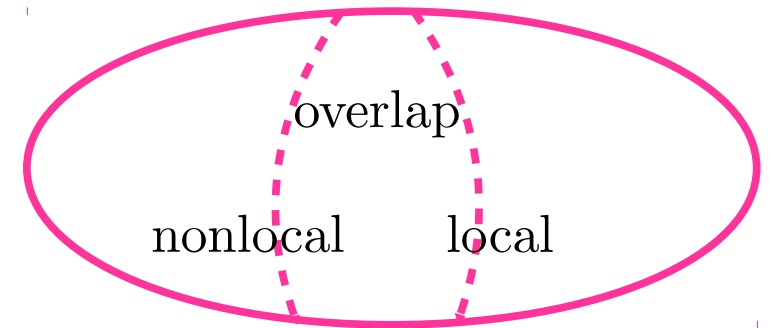
WHAT ABOUT COUPLING?

- 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



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- 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

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 $u(\mathbf{x}): \mathbb{R}^d \rightarrow \mathbb{R}$ and $\boldsymbol{\nu}(\mathbf{x}, \mathbf{y}): \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}^d$

- divergence of $\boldsymbol{\nu}$: $\mathcal{D}(\boldsymbol{\nu})(\mathbf{x}) = \int_{\mathbb{R}^n} (\boldsymbol{\nu}(\mathbf{x}, \mathbf{y}) + \boldsymbol{\nu}(\mathbf{y}, \mathbf{x})) \cdot \boldsymbol{\alpha}(\mathbf{x}, \mathbf{y}) d\mathbf{y}$

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

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

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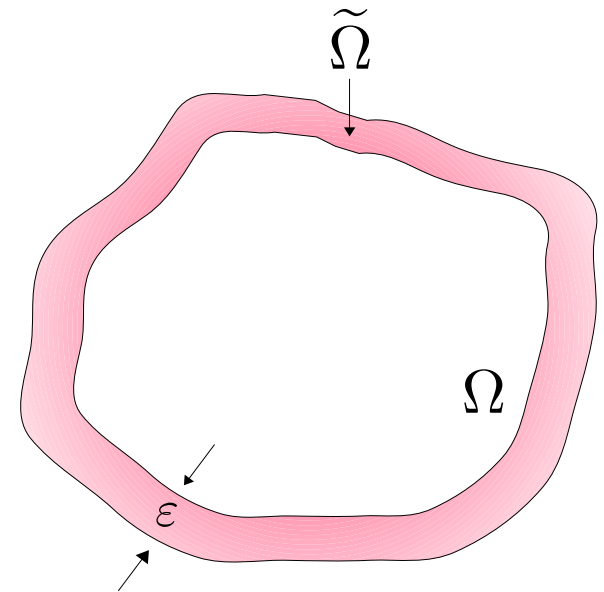
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NONLOCAL VECTOR CALCULUS

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

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

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

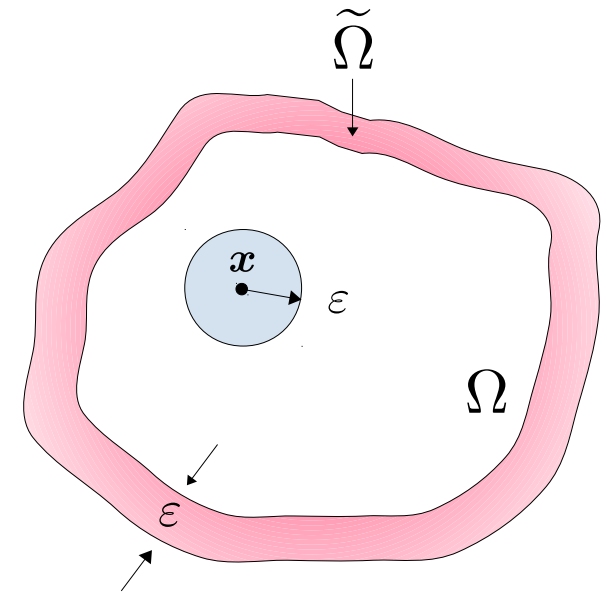


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Kernel: we assume

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

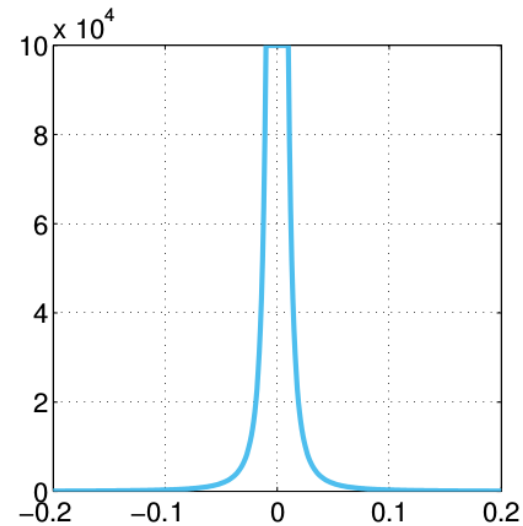
$$B_\varepsilon(\mathbf{x}) = \{\mathbf{y} \in \Omega^+ : |\mathbf{x} - \mathbf{y}| < \varepsilon, \mathbf{x} \in \Omega\}$$

NONLOCAL VECTOR CALCULUS

Example: for $s \in (0, 1)$

$$\gamma(\mathbf{x}, \mathbf{y}) = \frac{\gamma_1}{|\mathbf{y} - \mathbf{x}|^{n+2s}} \quad \forall \mathbf{y} \in B_\varepsilon(\mathbf{x})$$

$$V(\Omega^+) \sim H^s(\Omega^+)$$



M. D'Elia, M. Gunzburger, Computers and Mathematics with applications, 2013

THE LtN OPTIMIZATION PROBLEM

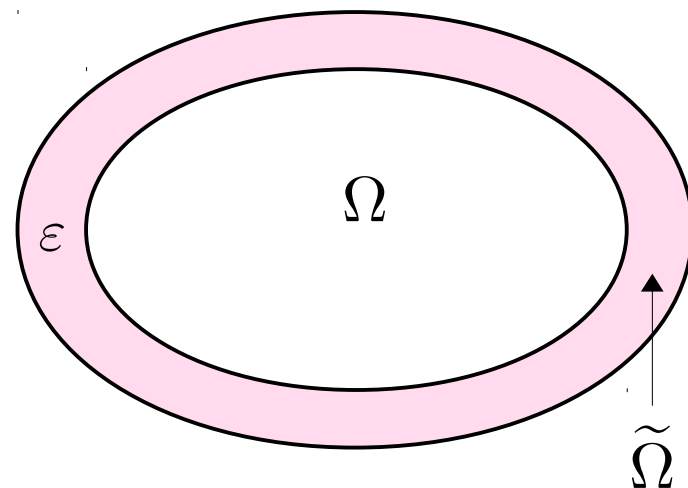
- M. D'Elia, P. Bochev, Optimization-Based Coupling of Nonlocal and Local Diffusion Models, *Materials Research Society Proceedings*, 2014
- M. D'Elia, P. Bochev, Formulation, Analysis and Computation of an optimization-based Local-to-Nonlocal Coupling Method, 2015

MODEL PROBLEMS

The nonlocal problem

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

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

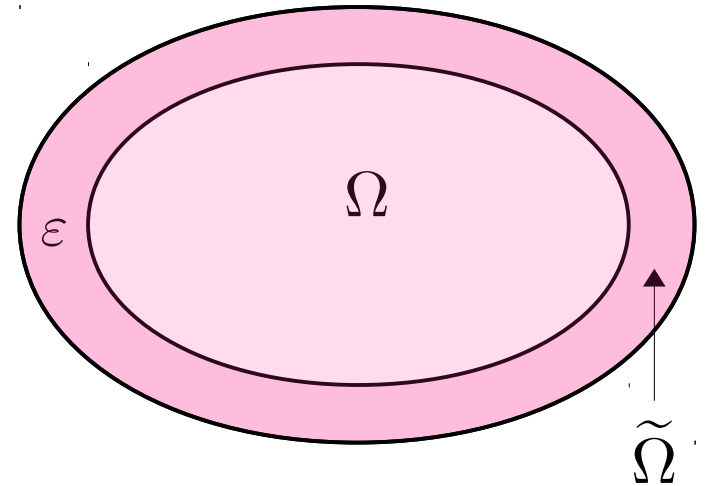


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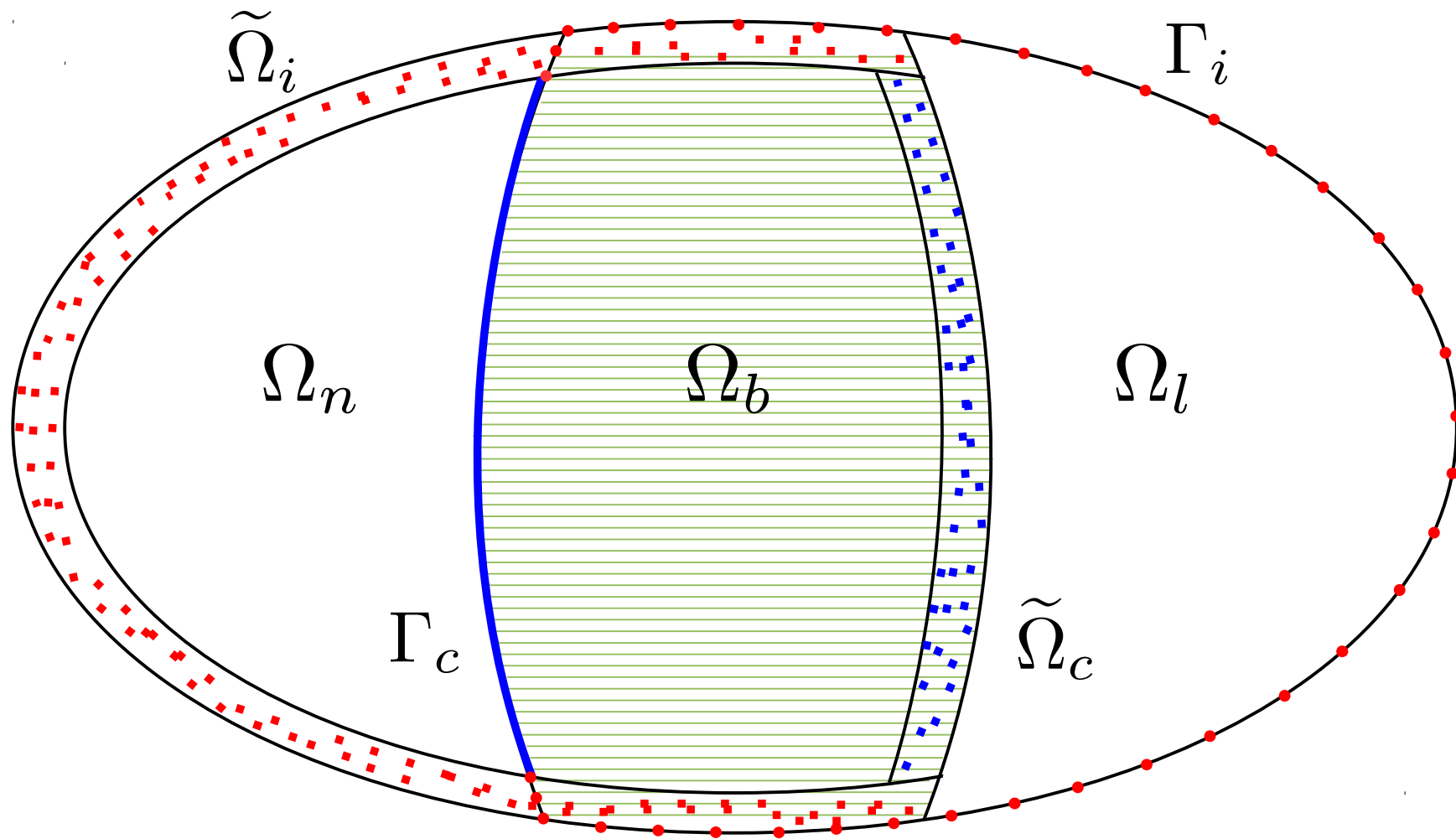
The local problem

local diffusion model given by the Poisson equation

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

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

LtN COUPLING



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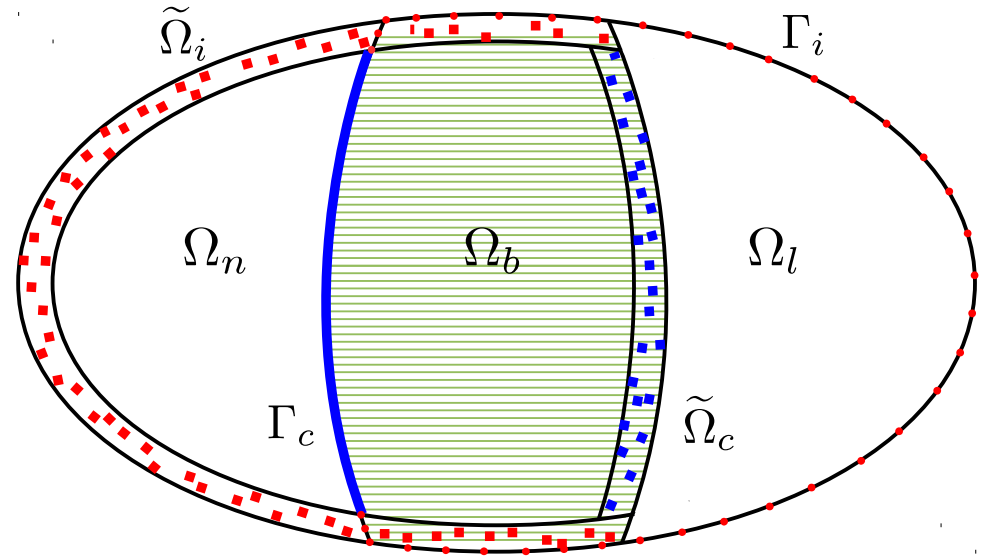
Notation:

$$\Omega_n^+ := \Omega_n \cup \tilde{\Omega}_n \subset \Omega^+$$

$$\Omega_b = \Omega_n^+ \cap \Omega_l \neq \emptyset$$

$$\tilde{\Omega}_n = \tilde{\Omega}_i \cup \tilde{\Omega}_c$$

$$\partial\Omega_l = \Gamma_i \cup \Gamma_c$$



LtN COUPLING

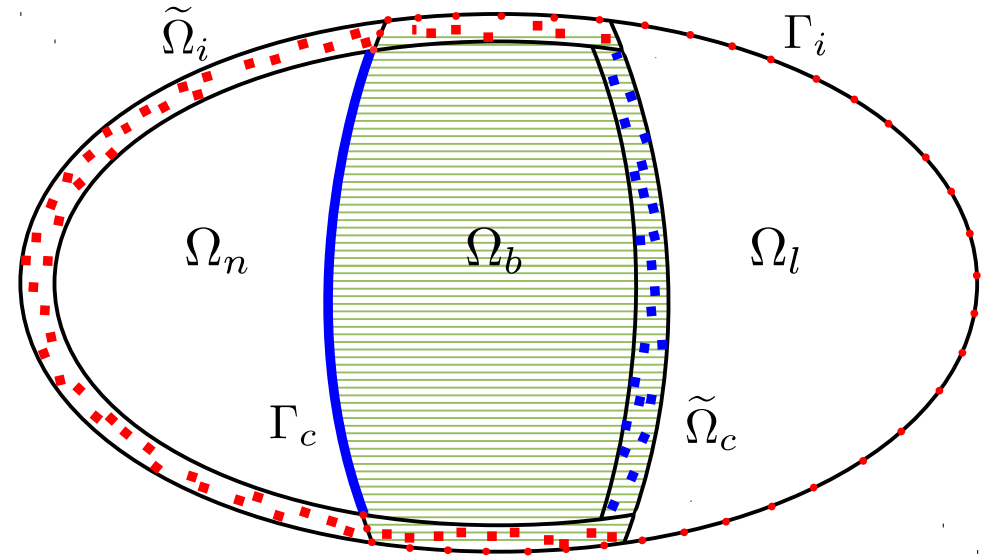
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State equations:

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

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

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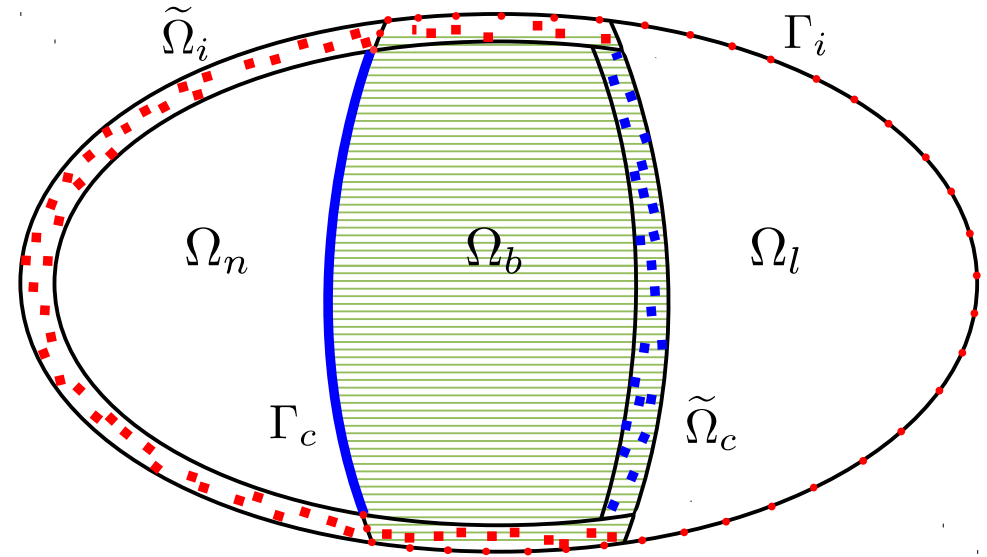
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Optimization problem:

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

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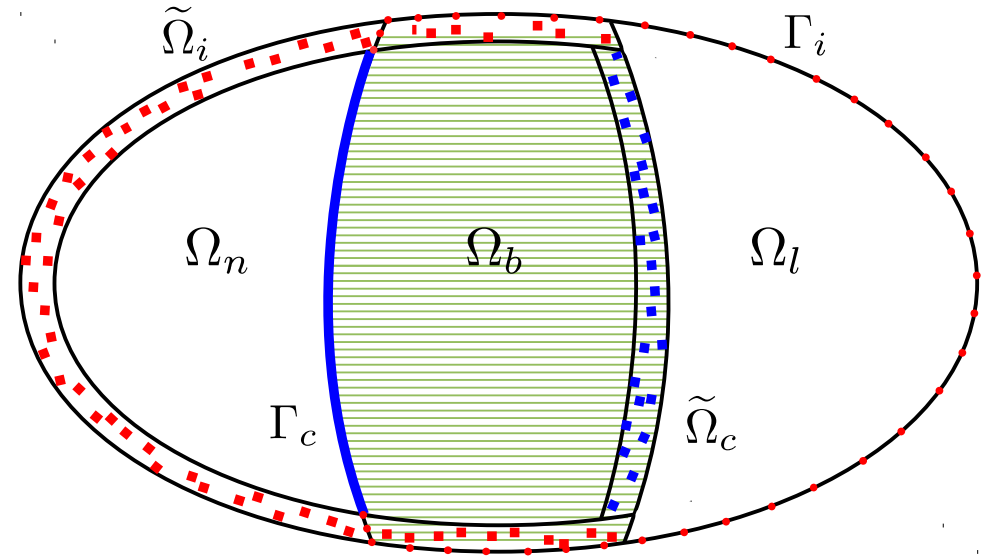
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control variables $(\theta_n, \theta_l) \in \Theta_n \times \Theta_l = \{(\sigma_n, \sigma_l) : \sigma_n \in \tilde{V}_{\tilde{\Omega}_i}(\tilde{\Omega}_c), \sigma_l \in H^{\frac{1}{2}}(\Gamma_c)\}$

LtN COUPLING

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

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

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Questions: • is it unique?

• what is the “error” wrt the global nonlocal solution $\hat{u}_n$?

$$\begin{cases} -\mathcal{L}\hat{u}_n & = & f & \mathbf{x} \in \Omega \\ \hat{u}_n & = & 0 & \mathbf{x} \in \tilde{\Omega} \end{cases}$$

IS THE SOLUTION UNIQUE?

Reduced form:

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

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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

$$\left\{ \begin{array}{lll} -\mathcal{L}v_n & = 0 & \mathbf{x} \in \Omega_n \\ v_n & = \theta_n & \mathbf{x} \in \tilde{\Omega}_c \\ v_n & = 0 & \mathbf{x} \in \tilde{\Omega}_i \end{array} \right. \quad \text{and} \quad \left\{ \begin{array}{lll} -\Delta v_l & = 0 & \mathbf{x} \in \Omega_l \\ v_l & = \theta_l & \mathbf{x} \in \Gamma_c \\ v_l & = 0 & \mathbf{x} \in \Gamma_i \end{array} \right.$$

homogeneous components u_n^0 and u_l^0

$$\left\{ \begin{array}{lll} -\mathcal{L}u_n^0 & = f_n & \mathbf{x} \in \Omega_n \\ u_n^0 & = 0 & \mathbf{x} \in \tilde{\Omega}_n \end{array} \right. \quad \text{and} \quad \left\{ \begin{array}{lll} -\Delta u_l^0 & = f_l & \mathbf{x} \in \Omega_l \\ u_l^0 & = 0 & \mathbf{x} \in \partial\Omega_l \end{array} \right.$$

IS THE SOLUTION UNIQUE?

Reduced functional:

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

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

IS THE SOLUTION UNIQUE? WELL-POSEDNESS/CONVEXITY

Reduced functional:

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

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

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

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

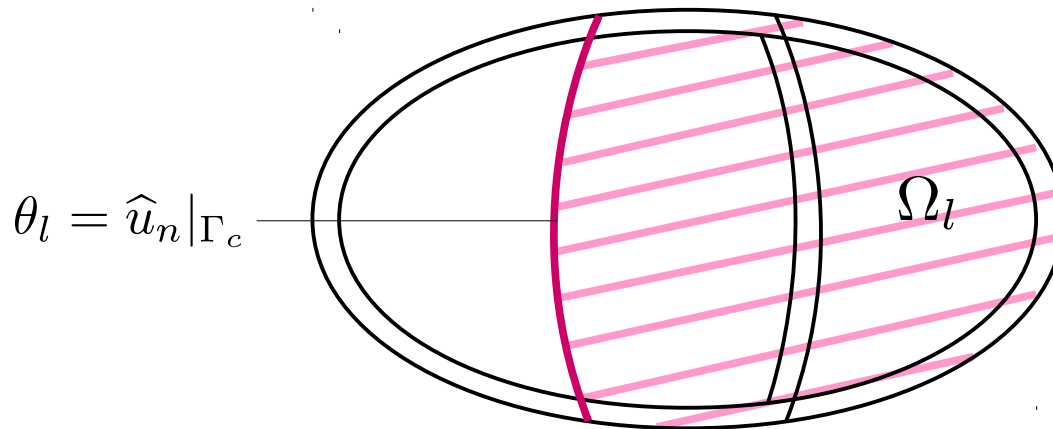
$\Rightarrow$ the functional J is **convex** wrt $\|(\cdot, \cdot)\|_*$

THE COUPLING ERROR

Coupling error $\leq C$ Modeling error

$$\|\hat{u}_n - u^*\|_{0,\Omega^+} \leq C \|\hat{u}_n - \hat{u}_l\|_{0,\Omega_l}$$

$\hat{u}_l$ solves the local problem in Ω_l with Dirichlet data $\theta_l = \hat{u}_n|_{\Gamma_c}$



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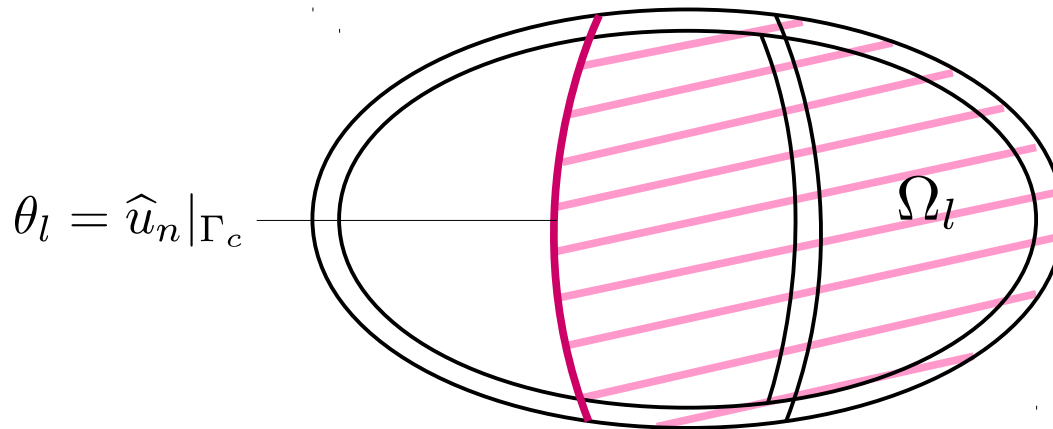
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Theorem: if $\Delta w - \mathcal{L}w \sim O(\varepsilon^2)$ for all $w \in C^4(\Omega_l)$,
then $\|\hat{u}_n - \hat{u}_l\|_{0,\Omega_l} \leq \tilde{C}\varepsilon^2 + O(\varepsilon^4)$

ASSUMPTIONS, LEMMAS AND TOOLS

Assumptions:

- $\bar{\gamma}_k = \|\gamma_k\|_\infty^{1/k} < \infty$ with $\gamma_k(\boldsymbol{x}) = \int_{\Omega^+} \gamma^k(\boldsymbol{x}, \boldsymbol{y}) d\boldsymbol{y}$, $k = 1, 2$
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- nonlocal trace inequality
- equivalence of L^2 norm and the nonlocal state space norm
- strong Cauchy-Schwarz inequality for the harmonic components

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Tools:

- nonlocal (and local) Poincaré inequality
- local Caccioppoli inequality for harmonic functions $\|\nabla v\|_{0, \bar{\Omega}} \leq C \|v\|_{0, \bar{\Omega}}$

FINITE DIMENSIONAL APPROXIMATION

- M. D'Elia, P. Bochev, Optimization-Based Coupling of Nonlocal and Local Diffusion Models, *Materials Research Society Proceedings*, 2014
- M. D'Elia, P. Bochev, Formulation, Analysis and Computation of an optimization-based Local-to-Nonlocal Coupling Method, 2015

THE ALGORITHM

Optimization problem:

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

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weak form + finite elements

(using the nonlocal vector calculus)

$$\int_{\Omega^+} \int_{\Omega^+} \mathcal{G}(u_n) \cdot \mathcal{G}(z_n) d\mathbf{y} d\mathbf{x} = \int_{\Omega} f_n z_n d\mathbf{x}$$

weak form + finite elements

$$\int_{\Omega_l} \nabla u_l \nabla z_l d\mathbf{x} = \int_{\Omega_l} f_l z_l d\mathbf{x}$$

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A gradient-based algorithm

Given an initial guess $\theta_{nh}^0, \theta_{lh}^0$, for $k = 0, 1, 2, \dots$

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

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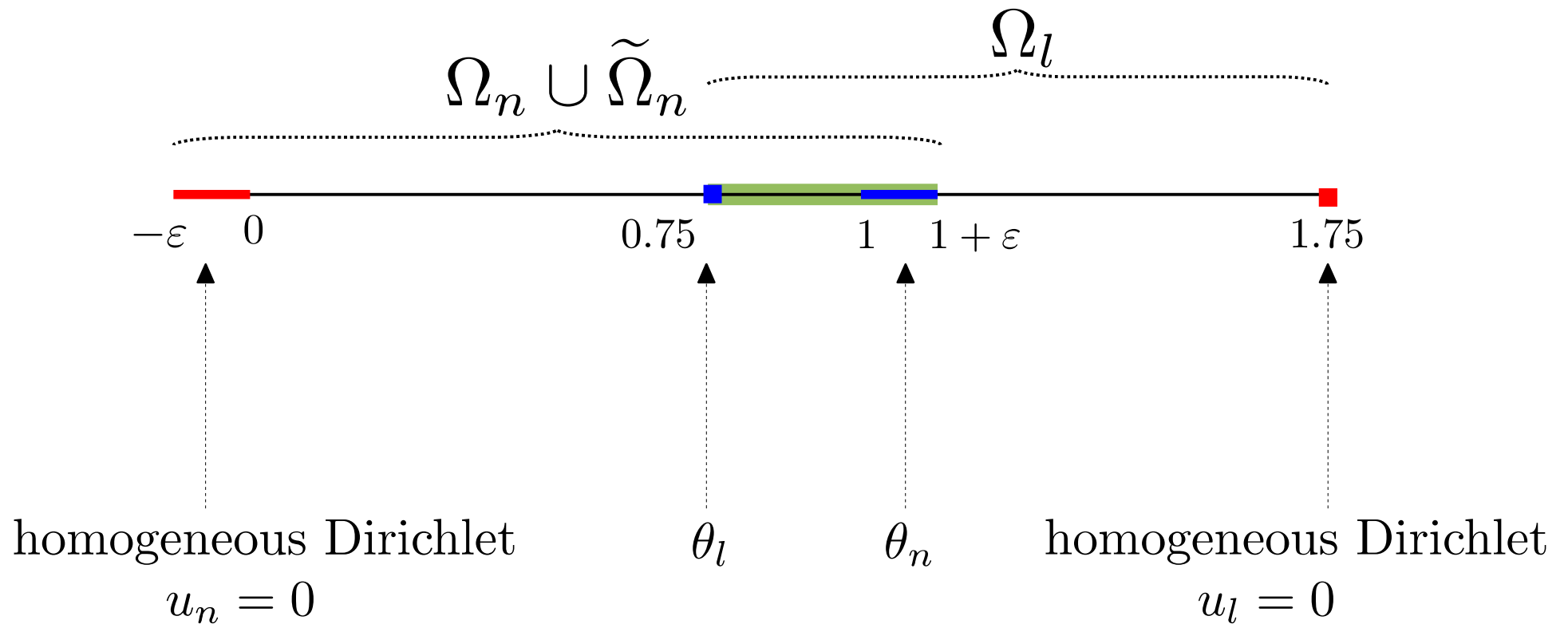
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NUMERICAL TESTS

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PROBLEM SETTING (1D)



NUMERICAL TESTS

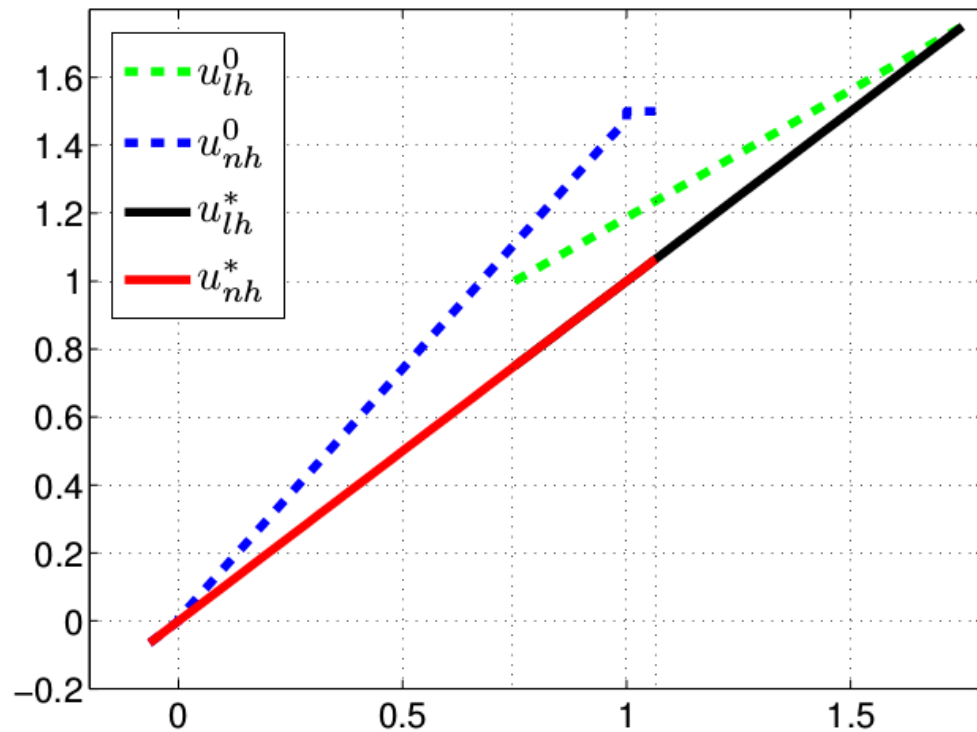
Kernel: $\gamma(x, y) = \frac{1}{\varepsilon^2 |x - y|} \chi(x - \varepsilon, x + \varepsilon)$

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The patch test:

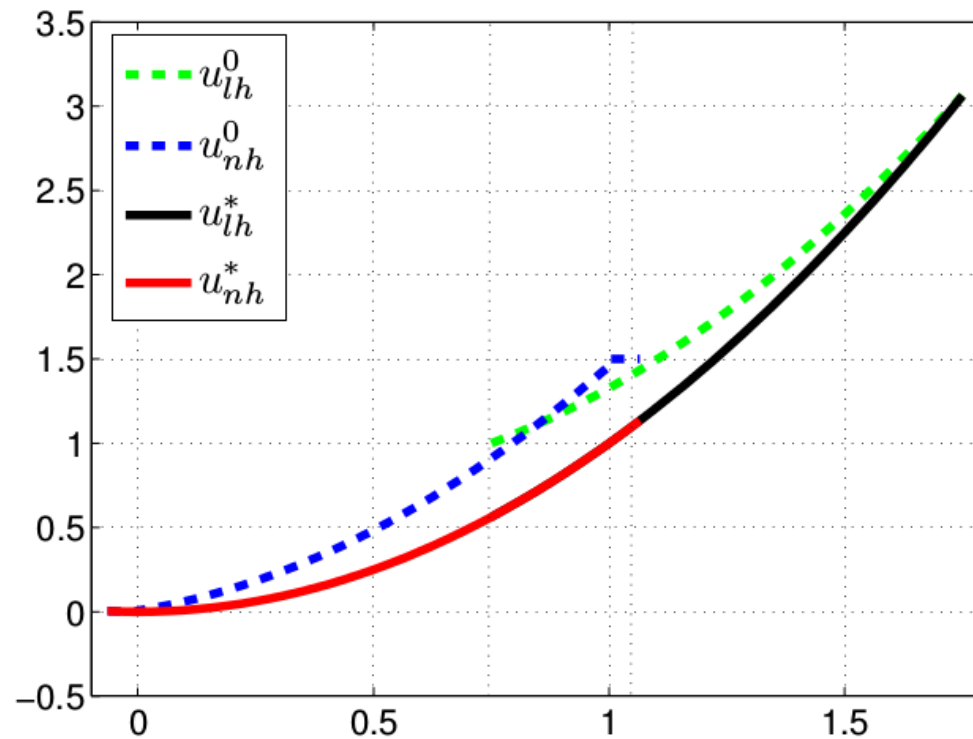
- $u_n = u_l = x$
- $u_n|_{\tilde{\Omega}_i} = x$
- $u_l(1.75) = 1.75$
- $f_n = f_l = 0$



NUMERICAL TESTS

Accuracy tests:

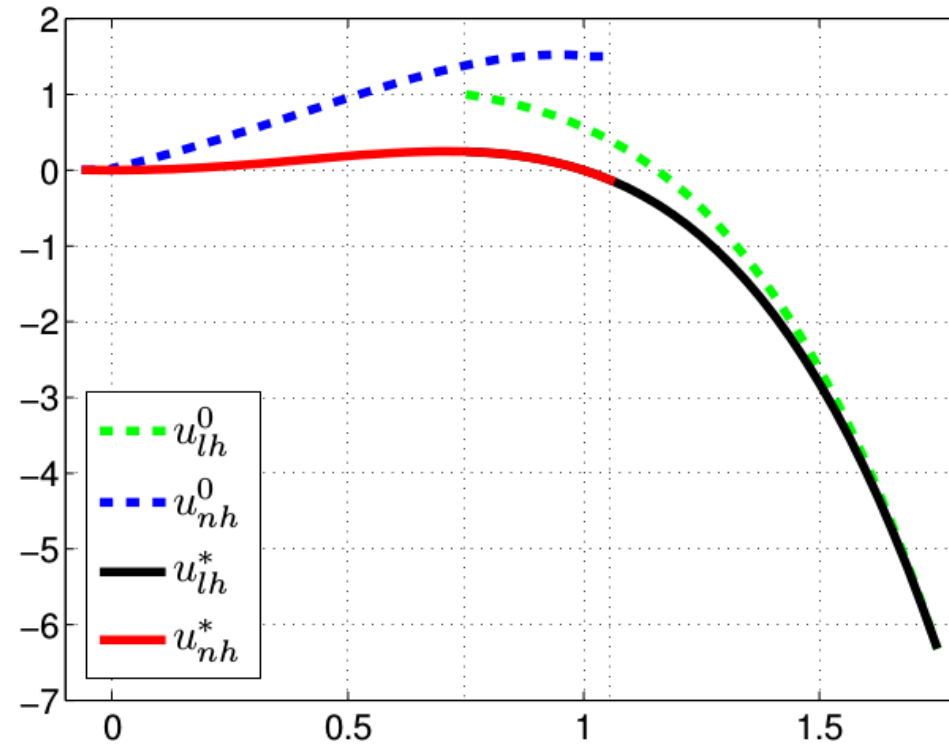
- $u_n = u_l = x^2$
 - $u_n|_{\tilde{\Omega}_i} = x^2$
 - $u_l(1.75) = 1.75^2$
 - $f_n = f_l = -2$



NUMERICAL TESTS

Accuracy tests:

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



NUMERICAL TESTS

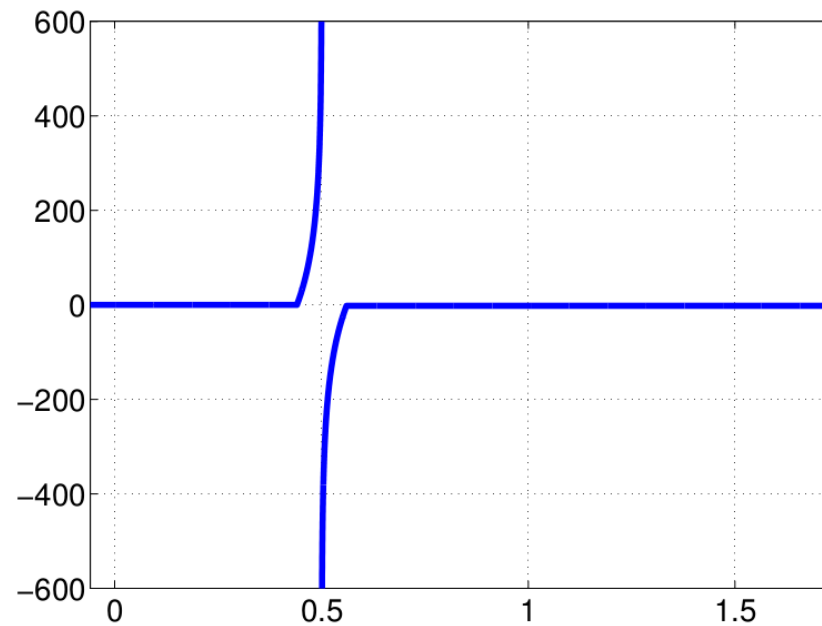
Accuracy tests:

	ε	h	$e(u_n)$	rate	$e(u_l)$	rate	$e(\theta_n)$	rate
test 1.	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
test 2.	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

NUMERICAL TESTS

More tests:

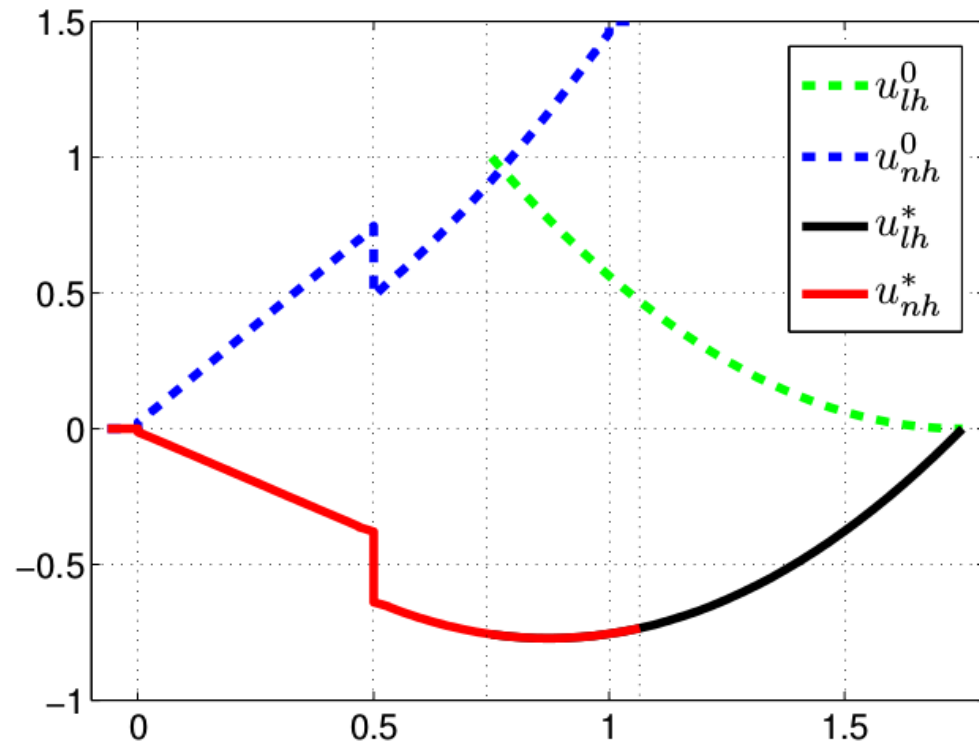
3. • $u_n|_{\tilde{\Omega}_i} = 0$
• $u_l(1.75) = 0$



NUMERICAL TESTS

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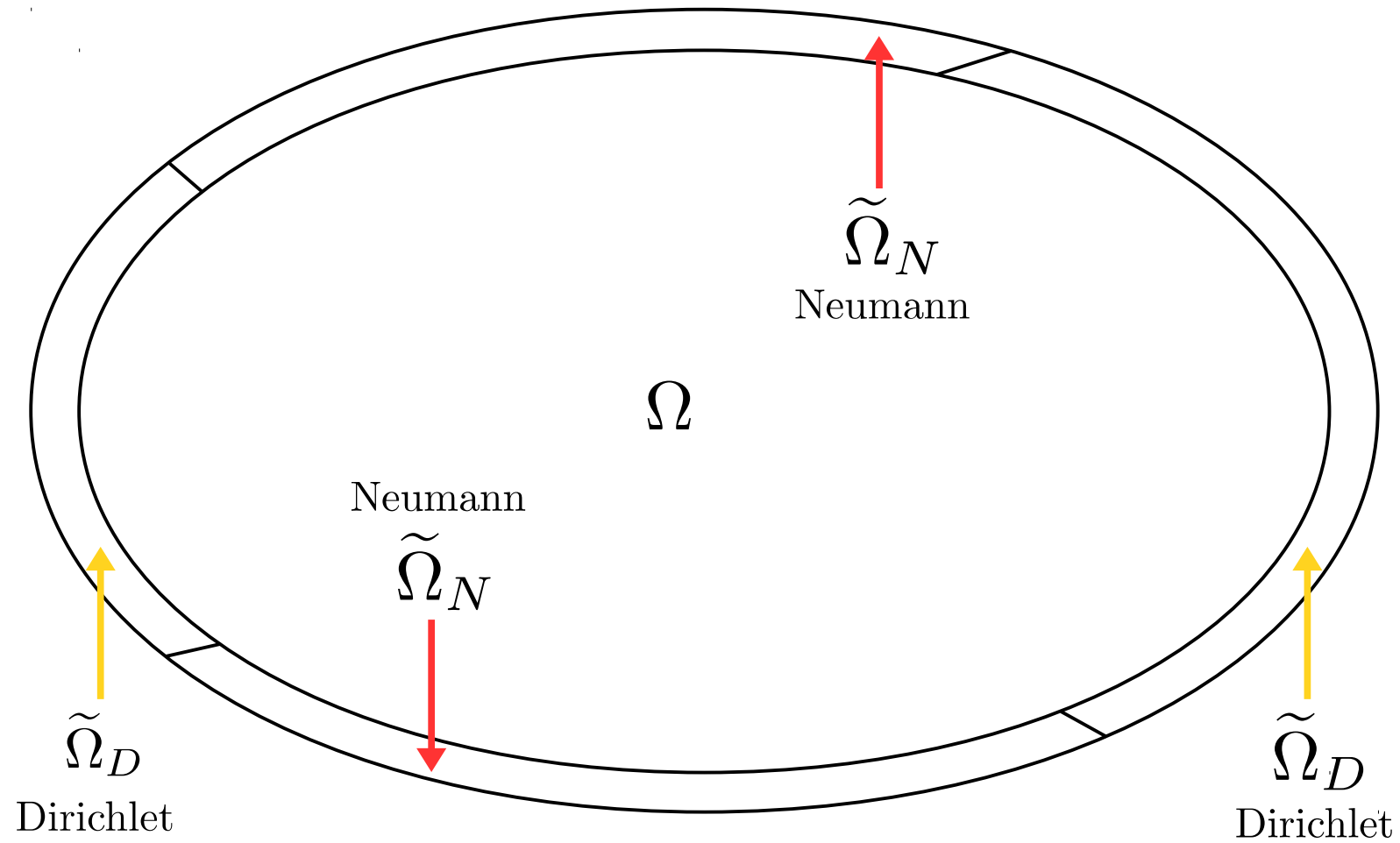
3. • $u_n|_{\tilde{\Omega}_i} = 0$
• $u_l(1.75) = 0$



CURRENT WORK

- Consider mixed boundary/volume value problems
- Do computational tests on 3D problems coupling Sandia's software
- Consider more general operators

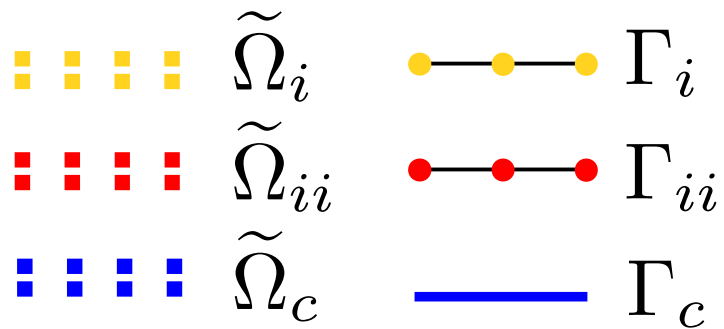
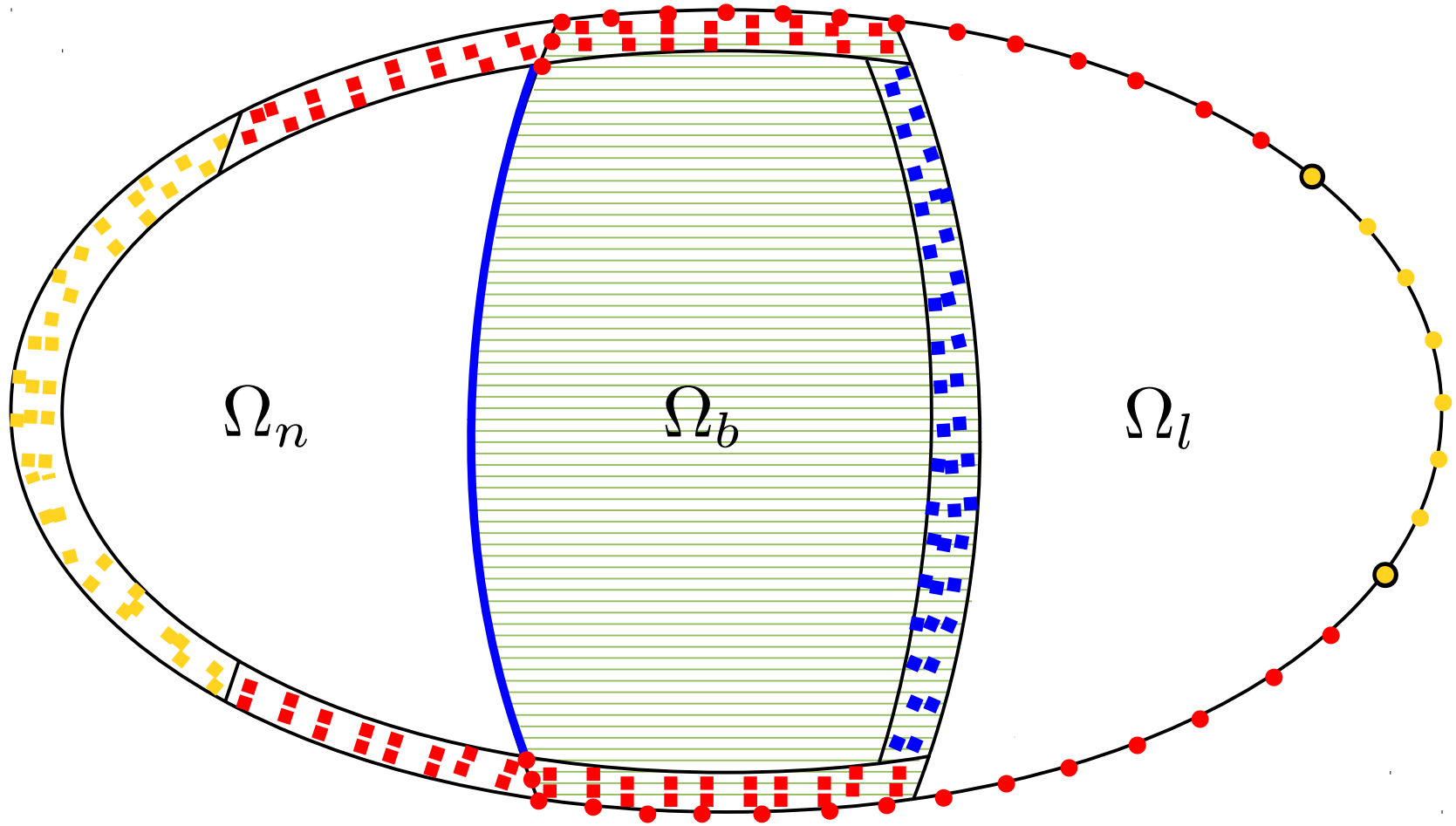
MIXED BOUNDARY/VOLUME VALUE PROBLEM



Dirichlet: prescribed displacement

Neumann: load force

MIXED BOUNDARY/VOLUME VALUE PROBLEM

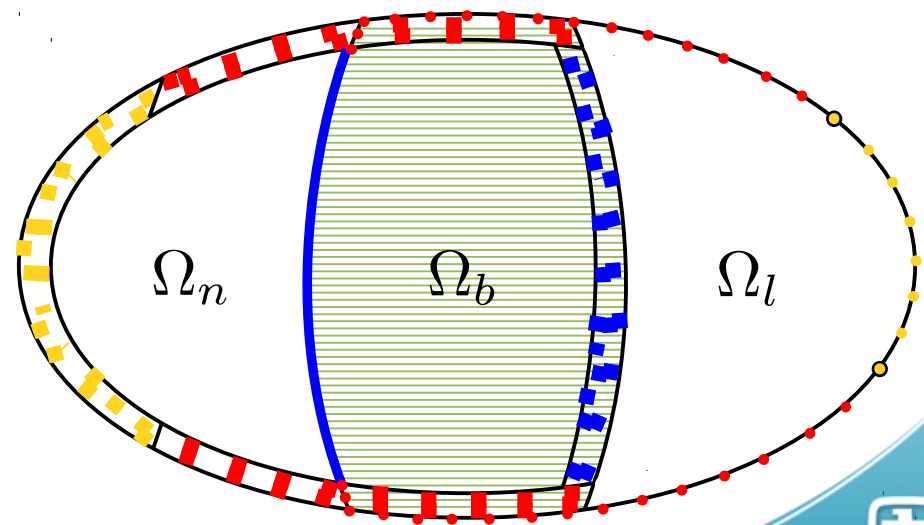


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control variables $(\theta_n, \theta_l) \in \Theta_n \times \Theta_l = \{(\sigma_n, \sigma_l) : \sigma_n \in \tilde{V}_{\tilde{\Omega}_i}(\tilde{\Omega}_c), \sigma_l \in H^{\frac{3}{2}}(\Gamma_c)\}$



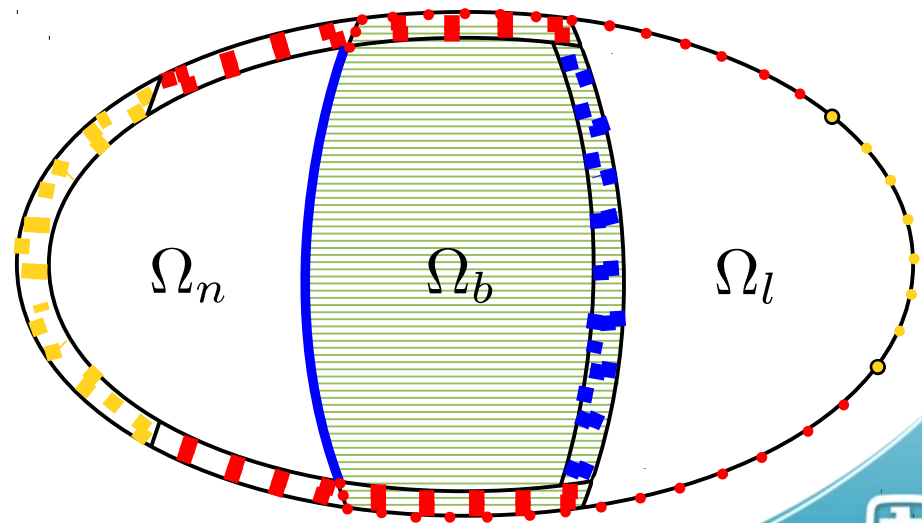
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Theorem: The reduced space problem has a unique solution



3D PROBLEM

Coupling Peridigm and Albany



peridigm.sandia.gov



software.sandia.gov/albany/

3D PROBLEM

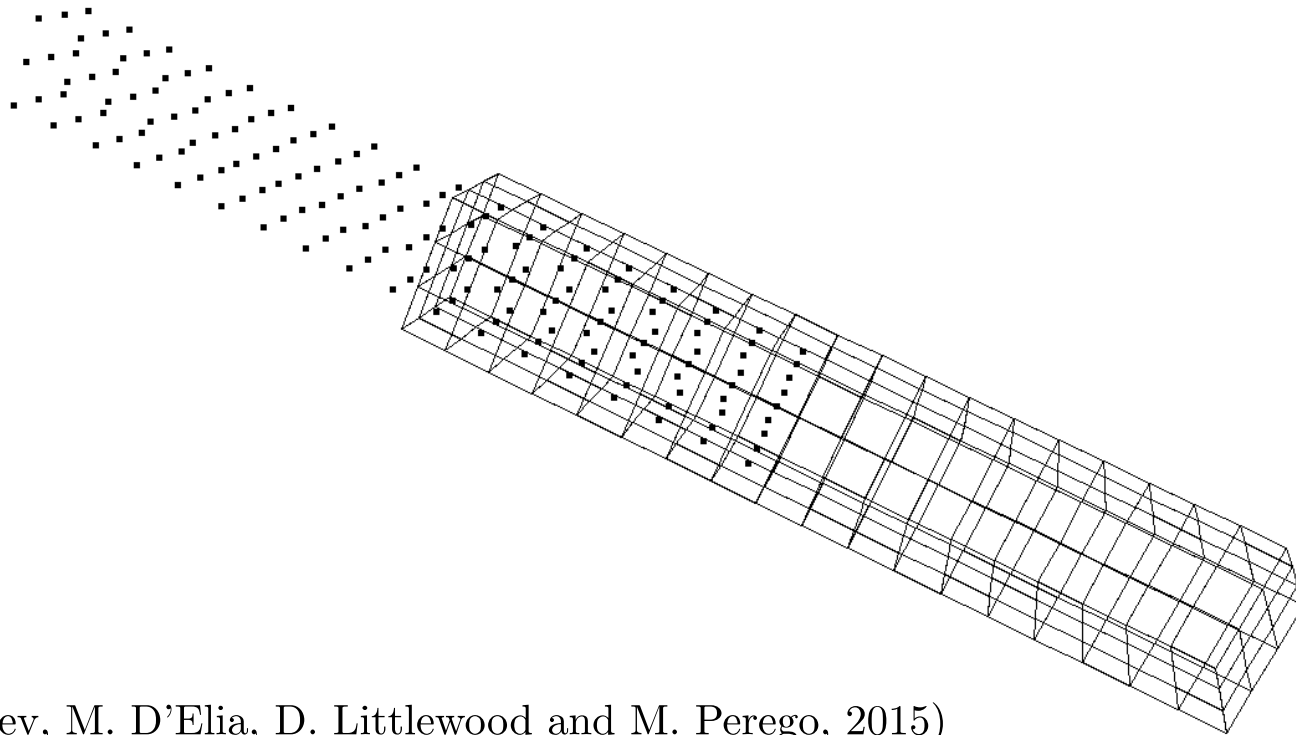
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(P. Bochev, M. D'Elia, D. Littlewood and M. Perego, 2015)

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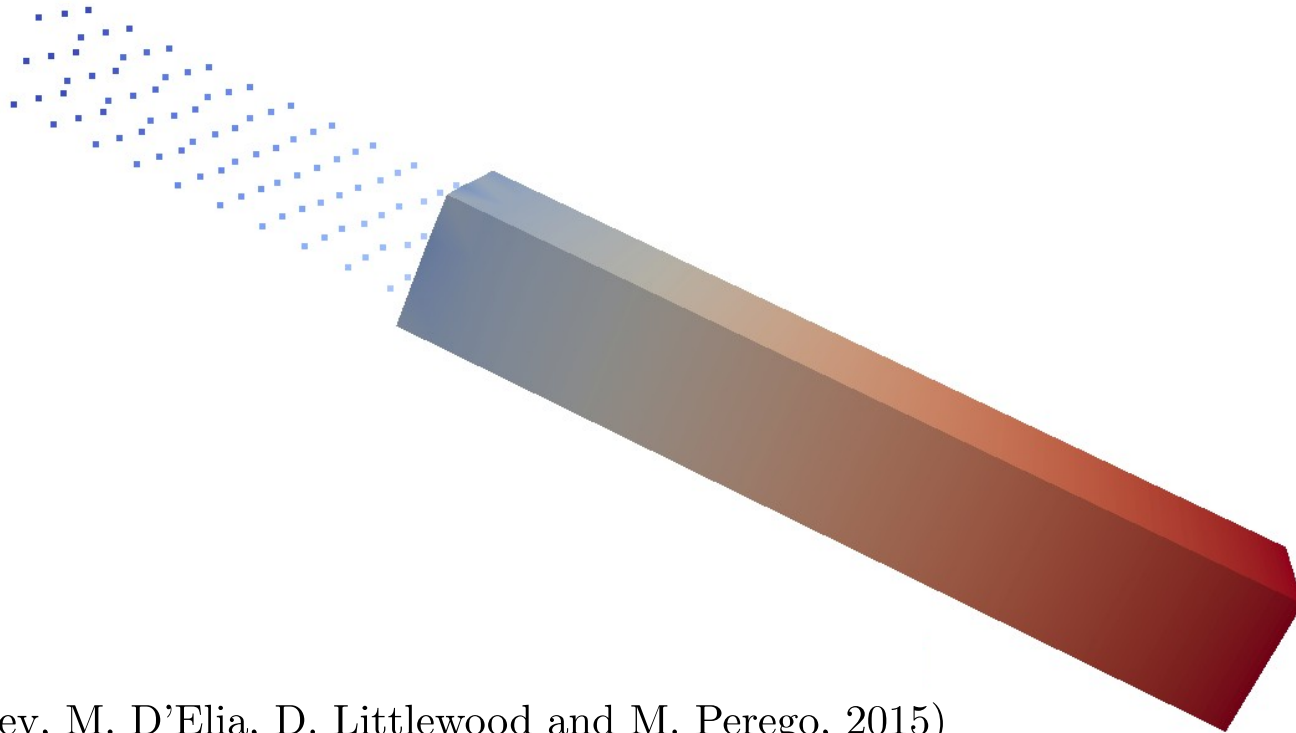
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Thank you