SAND2015-6511C

Formulation, Analysis and Computation of an Optimization–Based Local to Nonlocal coupling method

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

CCR
Center for Computing Research

Sandia National Labs, NM –

Sandia National Laboratories is a multi program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Sandia National Laboratories

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

NONLOCAL MODELS

nonlocal models are used in several diverse applications

our interest: nonlocal diffusion operators

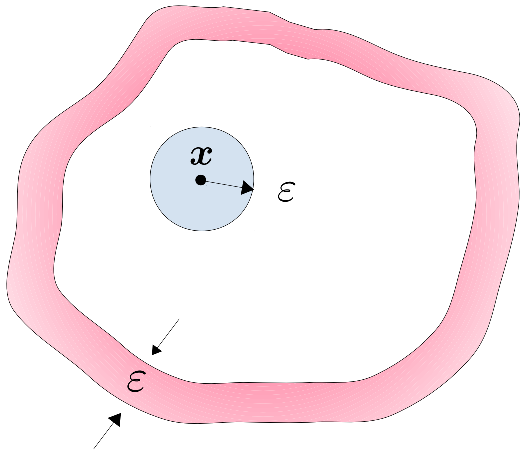
- peridynamic model for mechanics
- jump processes
- nonlocal heat conduction

how do they look like?

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

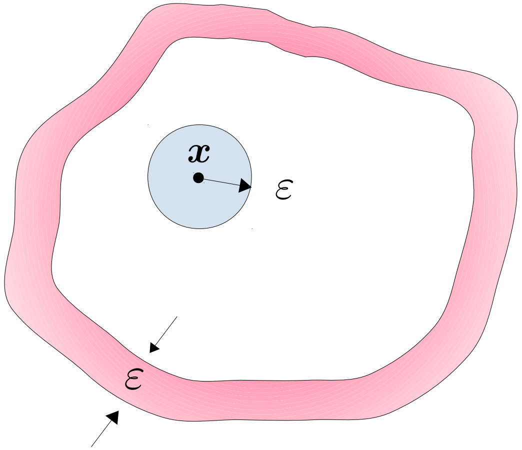
NONLOCAL MODELS

- 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

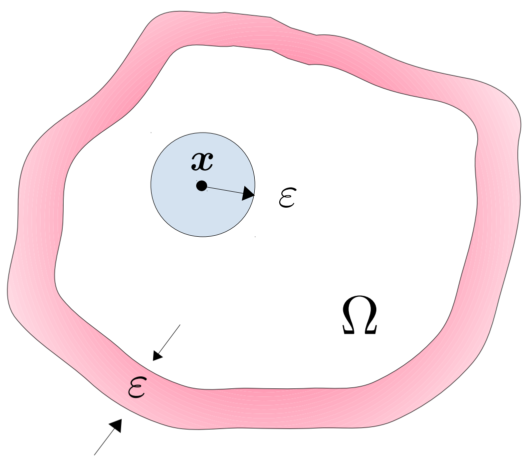


ductile fracture, Wikipedia

[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

- used to model stochastic jump processes, e.g. **Lévy jump processes** [1,2]
- **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

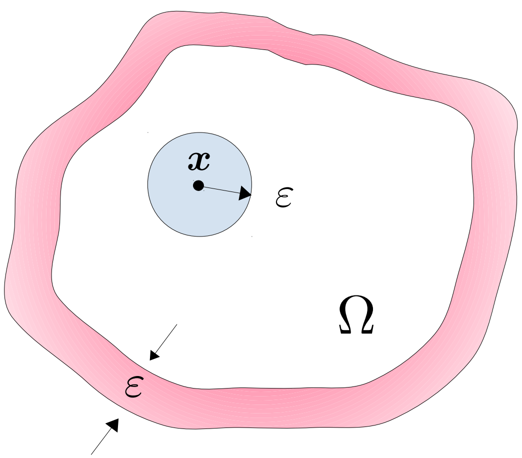
[2] O. Defterli, M. DElia, Q. Du, M. Gunzburger, R. Lehoucq, M.M. Meerschaert, Fractional Derivatives and Applications, 2015

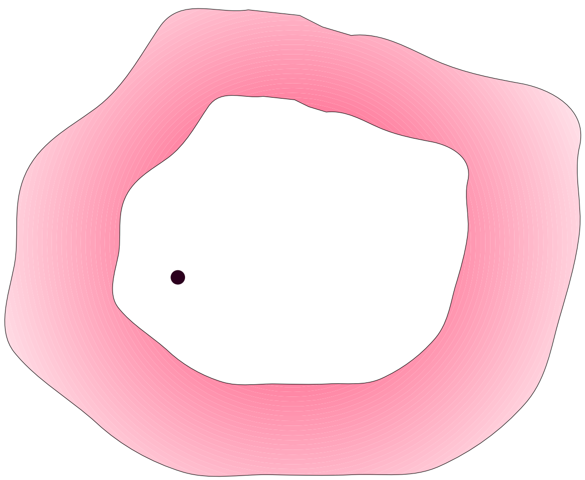
[3] N. Burch, M. D'Elia, R. Lehoucq, The European Physical Journal Special Topics, 2014

NONLOCAL MODELS

- used to model stochastic jump processes, e.g. **Lévy jump processes** [1,2]

- **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

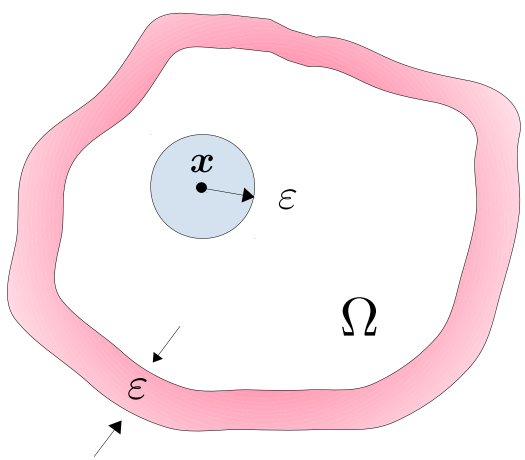
[2] O. Defterli, M. DElia, Q. Du, M. Gunzburger, R. Lehoucq, M.M. Meerschaert, Fractional Derivatives and Applications, 2015

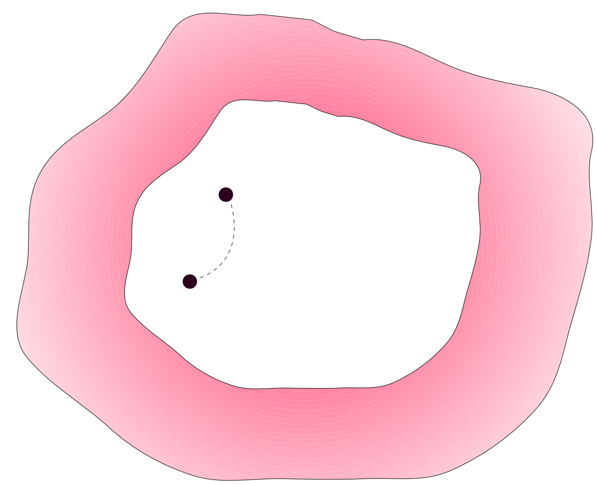
[3] N. Burch, M. D'Elia, R. Lehoucq, The European Physical Journal Special Topics, 2014

NONLOCAL MODELS

- used to model stochastic jump processes, e.g. **Lévy jump processes** [1,2]

- **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. DElia, Q. Du, M. Gunzburger, R. Lehoucq, M.M. Meerschaert, Fractional Derivatives and Applications, 2015

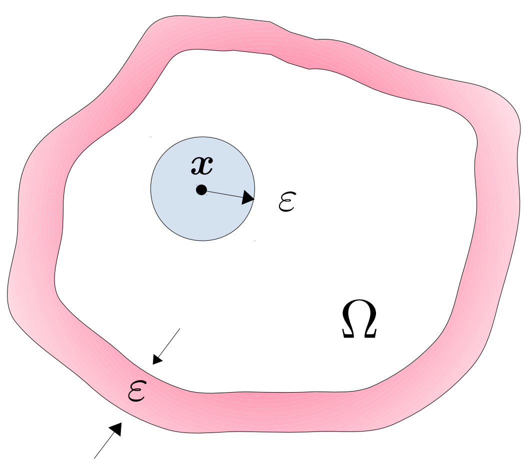
[3] N. Burch, M. D'Elia, R. Lehoucq, The European Physical Journal Special Topics, 2014

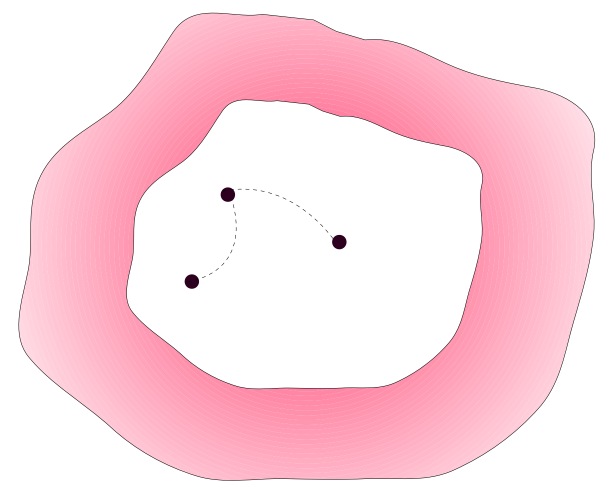
Sandia National Laboratories

NONLOCAL MODELS

- used to model stochastic jump processes, e.g. **Lévy jump processes** [1,2]

- **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

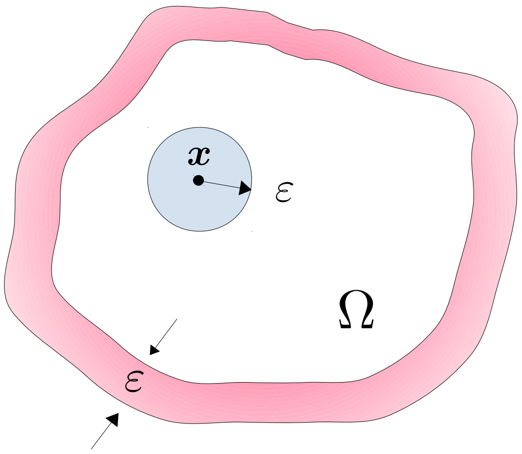
[2] O. Defterli, M. DElia, Q. Du, M. Gunzburger, R. Lehoucq, M.M. Meerschaert, Fractional Derivatives and Applications, 2015

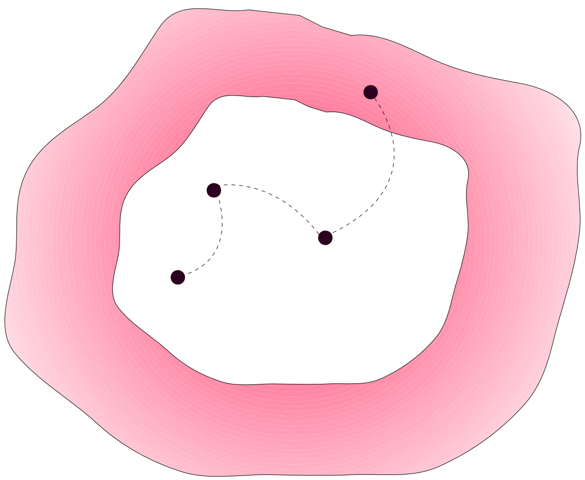
[3] N. Burch, M. D'Elia, R. Lehoucq, The European Physical Journal Special Topics, 2014

NONLOCAL MODELS

- used to model stochastic jump processes, e.g. **Lévy jump processes** [1,2]

- **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. DElia, 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

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:

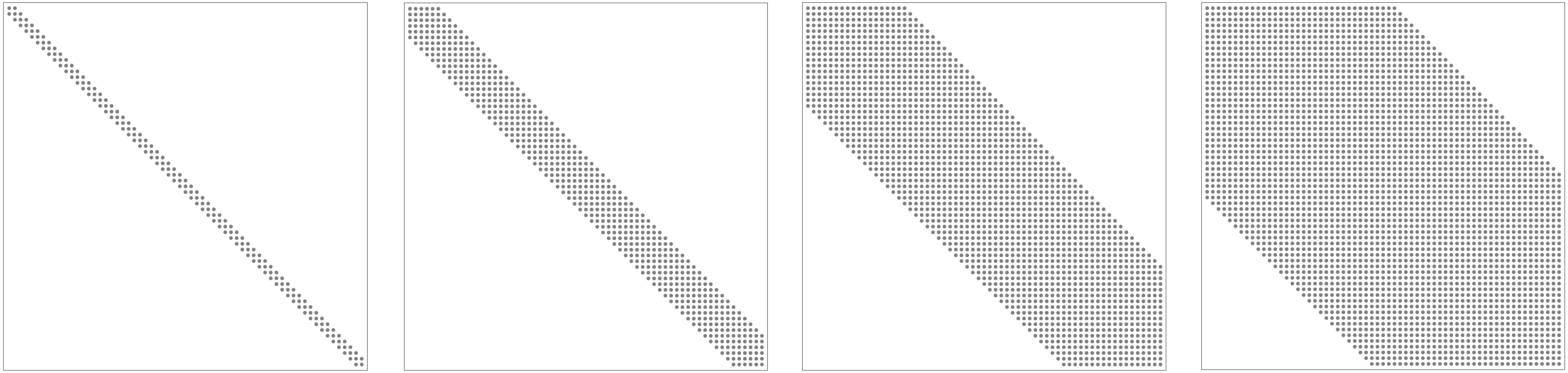
- the numerical solution of nonlocal models might be prohibitively expensive

- we can compute the solution of PDEs efficiently

NONLOCAL vs LOCAL

facts: • the numerical solution of nonlocal models might be prohibitively expensive

• we can compute the solution of PDEs efficiently

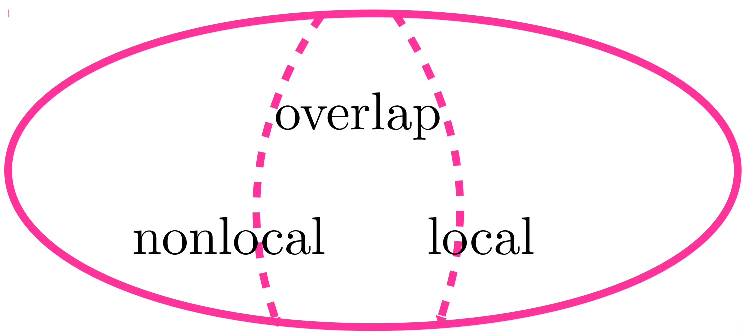


$\rightarrow$ increasing interaction radius $\rightarrow$

WHAT ABOUT COUPLING?

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

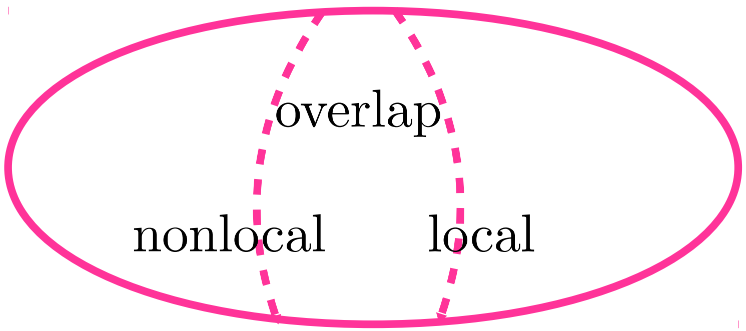
• split the computational domain in a local and a nonlocal domain and **couple**, in a smart way, the models at the interfaces or overlapping regions



WHAT ABOUT COUPLING?

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



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

NONLOCAL VECTOR CALCULUS

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

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

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

Sandia National Laboratories

NONLOCAL VECTOR CALCULUS

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

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

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

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

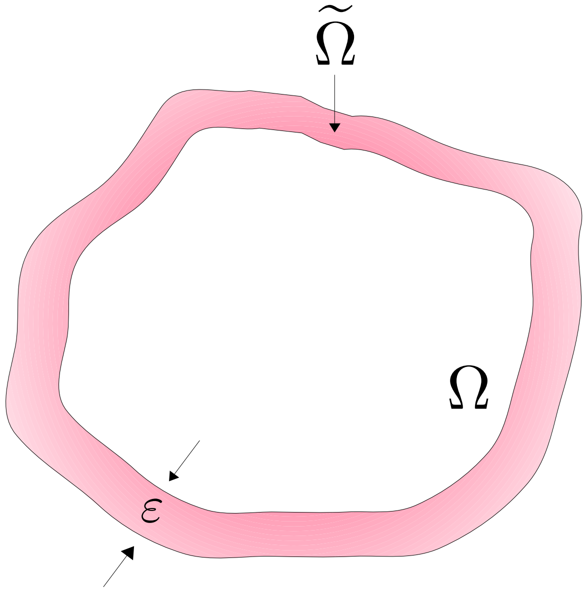
M. D'Elia – mdelia@sandia.gov

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

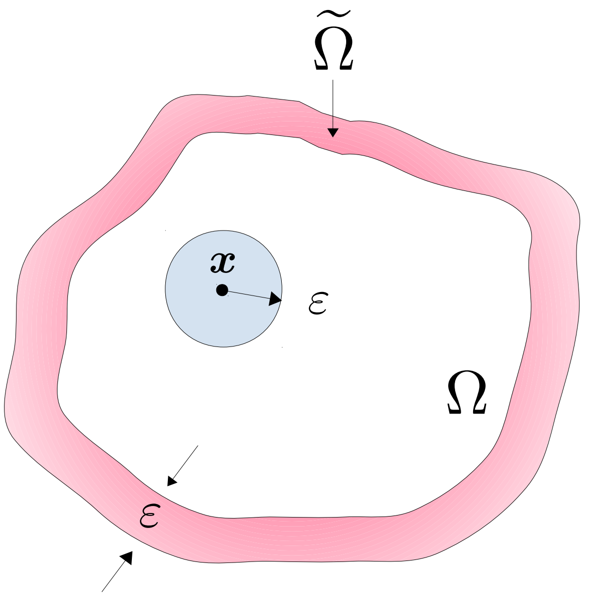


NONLOCAL VECTOR CALCULUS

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



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, P. Bochev, Optimization-Based Coupling of Nonlocal and Local Diffusion Models, *Materials Research Society Proceedings*, 2014

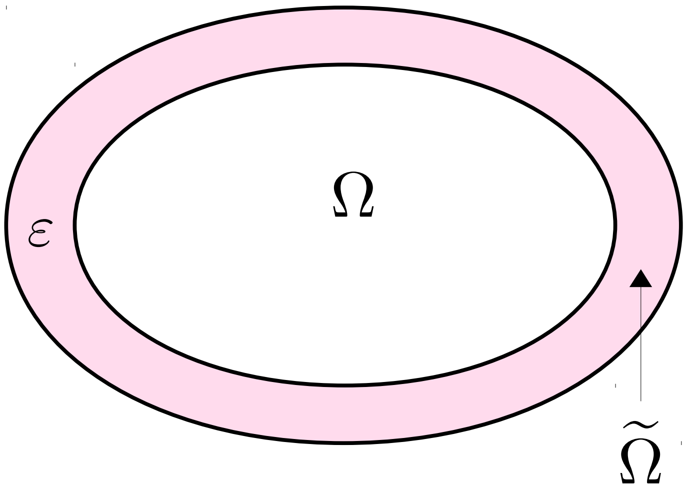
– M. D'Elia, P. Bochev, Formulation, Analysis and Computation of an optimization-based Local-to-Nonlocal Coupling Method, 2015

MODEL PROBLEMS

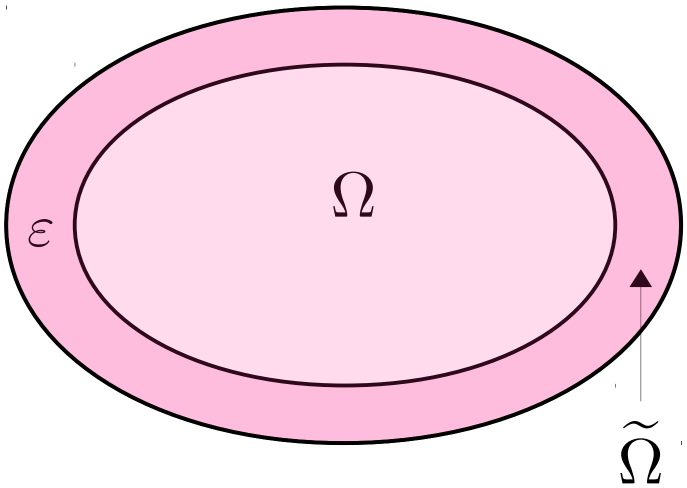
The nonlocal problem

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

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



MODEL PROBLEMS



The nonlocal problem

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

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

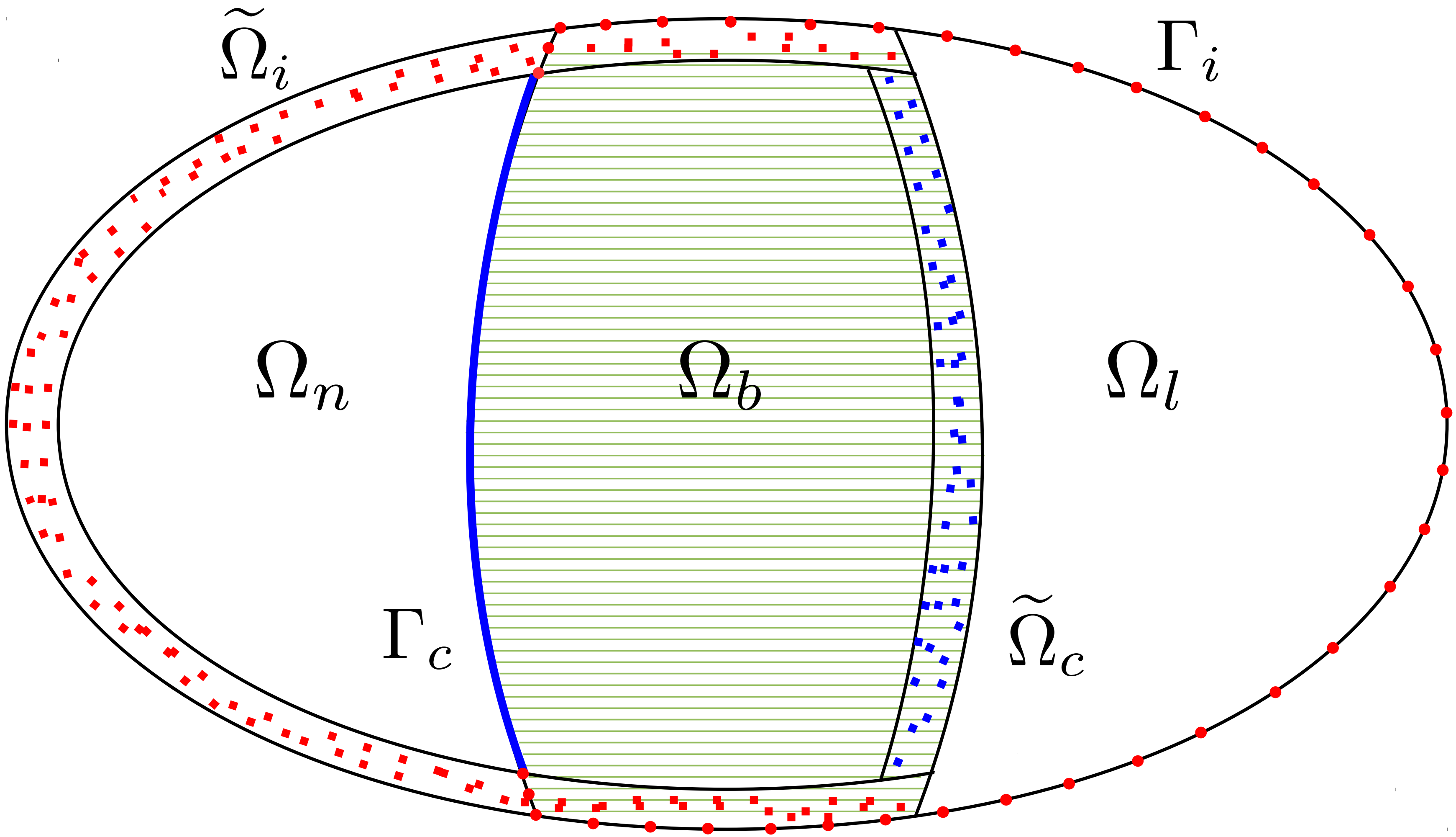
The local problem

local diffusion model given by the 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

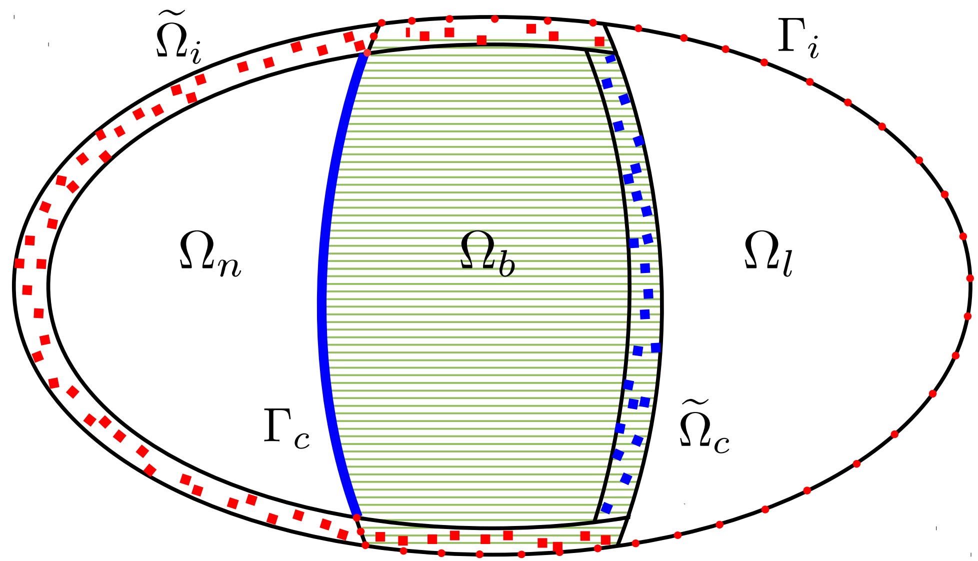
Notation:

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

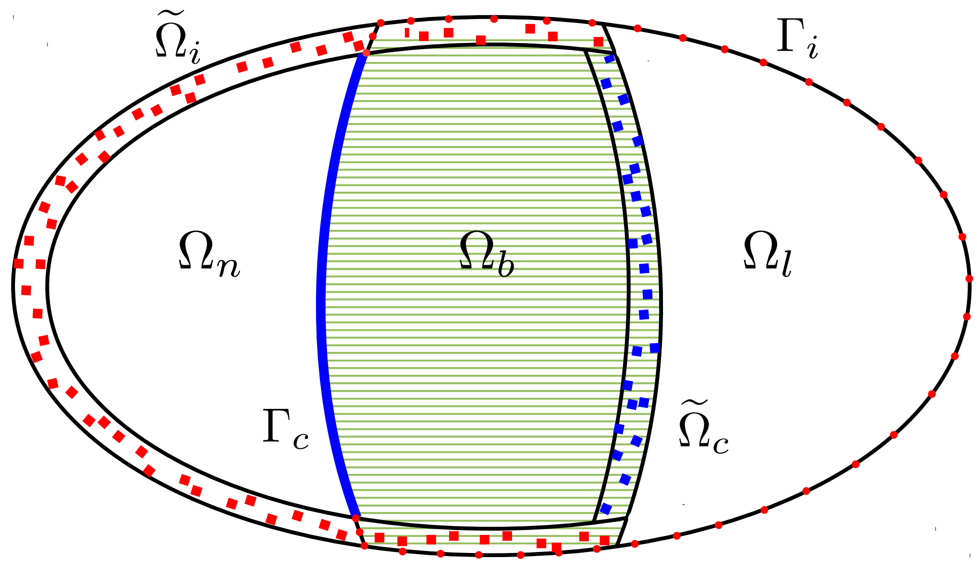
$$\Omega_b = \Omega_n^+ \cap \Omega_l \neq \emptyset$$

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

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



LtN COUPLING



Notation:

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

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

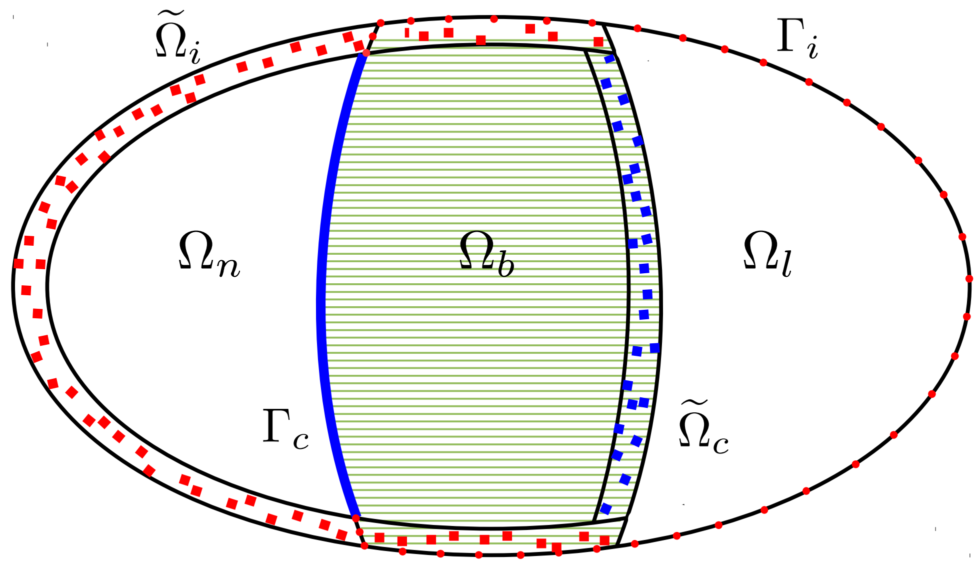
$$\widetilde{\Omega}_n = \widetilde{\Omega}_i \cup \widetilde{\Omega}_c$$

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

State equations:

$$\begin{cases} -\mathcal{L}u_n & = & f_n & \boldsymbol{x} \in \Omega_n \\ u_n & = & \theta_n & \boldsymbol{x} \in \widetilde{\Omega}_c \\ u_n & = & 0 & \boldsymbol{x} \in \widetilde{\Omega}_i \end{cases} \qquad \begin{cases} -\Delta u_l & = & f_l & \boldsymbol{x} \in \Omega_l \\ u_l & = & \theta_l & \boldsymbol{x} \in \Gamma_c \\ u_l & = & 0 & \boldsymbol{x} \in \Gamma_i. \end{cases}$$

LtN COUPLING



Notation:

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

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

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

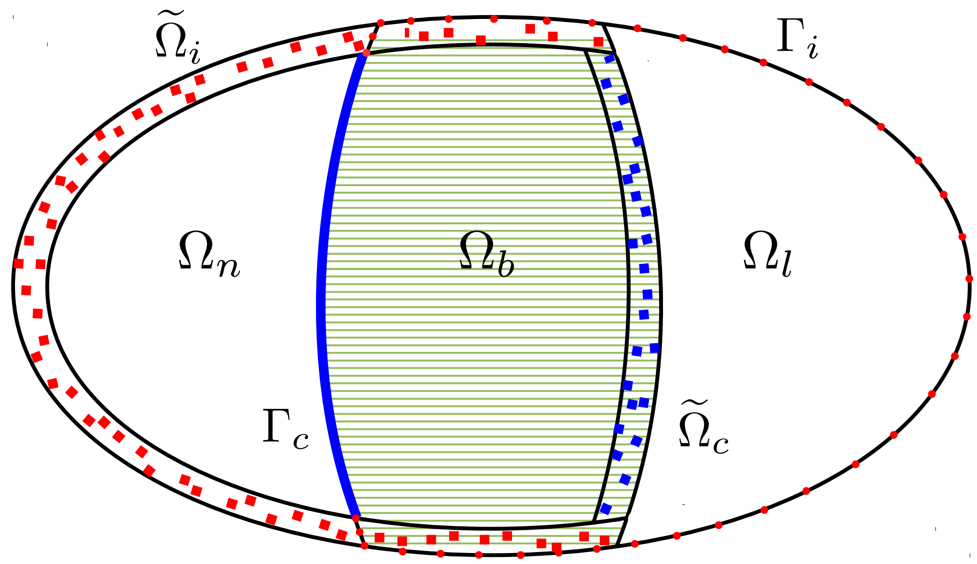
$$\partial\Omega_l = \Gamma_i \cup \Gamma_c$$

Optimization problem:

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

$$\text{s.t.} \quad \left\{ \begin{array}{rcll} -\mathcal{L}u_n & = & f_n & \boldsymbol{x} \in \Omega_n \\ u_n & = & \theta_n & \boldsymbol{x} \in \widetilde{\Omega}_c \\ u_n & = & 0 & \boldsymbol{x} \in \widetilde{\Omega}_i \end{array} \right. \qquad \left\{ \begin{array}{rcll} -\Delta u_l & = & f_l & \boldsymbol{x} \in \Omega_l \\ u_l & = & \theta_l & \boldsymbol{x} \in \Gamma_c \\ u_l & = & 0 & \boldsymbol{x} \in \Gamma_i. \end{array} \right.$$

LtN COUPLING



Notation:

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

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

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

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

Optimization problem:

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

$$\text{s.t.} \left\{ \begin{array}{rcll} -\mathcal{L}u_n & = & f_n & \boldsymbol{x} \in \Omega_n \\ u_n & = & \theta_n & \boldsymbol{x} \in \widetilde{\Omega}_c \\ u_n & = & 0 & \boldsymbol{x} \in \widetilde{\Omega}_i \end{array} \right. \qquad \left\{ \begin{array}{rcll} -\Delta u_l & = & f_l & \boldsymbol{x} \in \Omega_l \\ u_l & = & \theta_l & \boldsymbol{x} \in \Gamma_c \\ u_l & = & 0 & \boldsymbol{x} \in \Gamma_i. \end{array} \right.$$

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

LtN COUPLING

LtN solution

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

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

Questions:

- is it unique?

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

$$\begin{cases} -\mathcal{L}\widehat{u}_n = f & \boldsymbol{x} \in \Omega \\ \widehat{u}_n = 0 & \boldsymbol{x} \in \widetilde{\Omega} \end{cases}$$

IS THE SOLUTION UNIQUE?

Reduced form:

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

IS THE SOLUTION UNIQUE?

Reduced form:

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

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

$$\left\{\begin{aligned} -\mathcal{L}v_n &= 0 & \boldsymbol{x}\in\Omega_n \\ v_n &= \theta_n & \boldsymbol{x}\in\widetilde{\Omega}_c \\ v_n &= 0 & \boldsymbol{x}\in\widetilde{\Omega}_i \end{aligned}\right. \qquad \text{and} \qquad \left\{\begin{aligned} -\Delta v_l &= 0 & \boldsymbol{x}\in\Omega_l \\ v_l &= \theta_l & \boldsymbol{x}\in\Gamma_c \\ v_l &= 0 & \boldsymbol{x}\in\Gamma_i \end{aligned}\right.$$

homogeneous components u_n^0 and u_l^0

$$\left\{\begin{aligned} -\mathcal{L}u_n^0 &= f_n & \boldsymbol{x}\in\Omega_n \\ u_n^0 &= 0 & \boldsymbol{x}\in\widetilde{\Omega}_n \end{aligned}\right. \qquad \text{and} \qquad \left\{\begin{aligned} -\Delta u_l^0 &= f_l & \boldsymbol{x}\in\Omega_l \\ u_l^0 &= 0 & \boldsymbol{x}\in\partial\Omega_l \end{aligned}\right.$$

IS THE SOLUTION UNIQUE?

Reduced functional:

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

IS THE SOLUTION UNIQUE?

Reduced functional:

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

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

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

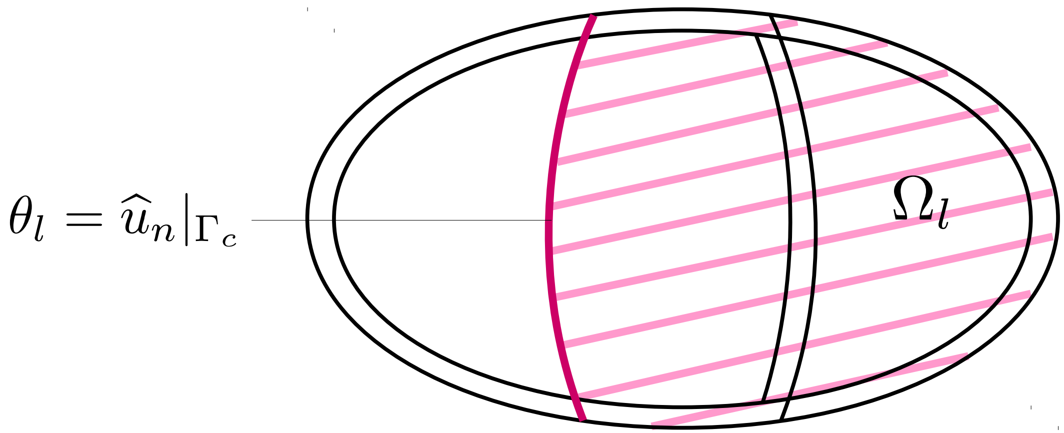
defines a norm in the control variable space

THE COUPLING ERROR

Coupling error $\leq C$ Modeling error

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

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



$$\begin{aligned} -\mathcal{L}\widehat{u}_n &= f \quad \boldsymbol{x} \in \Omega \\ \widehat{u}_n &= 0 \quad \boldsymbol{x} \in \widetilde{\Omega} \end{aligned}$$

$$\begin{aligned} -\Delta\widehat{u}_l &= f \quad && \boldsymbol{x} \in \Omega_l \\ \widehat{u}_l &= \widehat{u}_n|_{\Gamma_c} && \boldsymbol{x} \in \Gamma_c \\ \widehat{u}_l &= 0 && \boldsymbol{x} \in \Gamma_i \end{aligned}$$

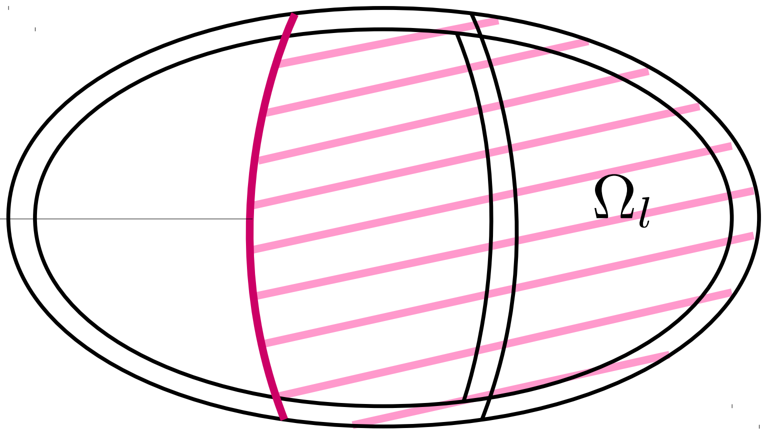
THE COUPLING ERROR

Coupling error $\leq C$ Modeling error

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

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

$\theta_l = \widehat{u}_n|_{\Gamma_c}$



$$\begin{aligned} -\mathcal{L}\widehat{u}_n &= f & \boldsymbol{x} \in \Omega \\ \widehat{u}_n &= 0 & \boldsymbol{x} \in \widetilde{\Omega} \end{aligned}$$

$$\begin{aligned} -\Delta\widehat{u}_l &= f & \boldsymbol{x} \in \Omega_l \\ \widehat{u}_l &= \widehat{u}_n|_{\Gamma_c} & \boldsymbol{x} \in \Gamma_c \\ \widehat{u}_l &= 0 & \boldsymbol{x} \in \Gamma_i \end{aligned}$$

Theorem: if $\Delta w - \mathcal{L}w \sim O(\varepsilon^2)$ for all $w \in C^4(\Omega_l)$,

then $\|\widehat{u}_n - \widehat{u}_l\|_{0,\Omega_l} \leq \widetilde{C}\varepsilon^2 + O(\varepsilon^4)$

ASSUMPTIONS, LEMMAS AND TOOLS

Assumptions:

- $\overline{\gamma}_k = \|\gamma_k\|_\infty^{1/k} < \infty \quad$ with $\quad \gamma_k(\boldsymbol{x}) = \int_{\Omega^+} \gamma^k(\boldsymbol{x}, \boldsymbol{y})\, d\boldsymbol{y}, \quad k = 1, 2$
- the global nonlocal solution has a trace on Γ_c

ASSUMPTIONS, LEMMAS AND TOOLS

Assumptions:

- $\overline{\gamma}_k = \|\gamma_k\|_\infty^{1/k} < \infty \quad \text{with} \quad \gamma_k(\boldsymbol{x}) = \int_{\Omega^+} \gamma^k(\boldsymbol{x},\boldsymbol{y})\, d\boldsymbol{y}, \quad k = 1,2$
- the global nonlocal solution has a trace on Γ_c

Lemmas:

- nonlocal trace inequality
- equivalence of L^2 norm and the nonlocal state space norm
- strong Cauchy-Schwarz inequality for the harmonic components

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

ASSUMPTIONS, LEMMAS AND TOOLS

Assumptions:

- $\overline{\gamma}_k = \|\gamma_k\|_\infty^{1/k} < \infty \quad \text{with} \quad \gamma_k(\boldsymbol{x}) = \int_{\Omega^+} \gamma^k(\boldsymbol{x},\boldsymbol{y})\, d\boldsymbol{y}, \quad k = 1,2$
- the global nonlocal solution has a trace on Γ_c

Lemmas:

- nonlocal trace inequality
- equivalence of L^2 norm and the nonlocal state space norm
- 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 (and local) Poincaré inequality
- local Caccioppoli inequality for harmonic functions $\|\nabla v\|_{0,\overline{\Omega}} \leq C\|v\|_{0,\overline{\Omega}}$

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:

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

$$\text{s.t.} \quad \left\{\begin{array}{rcll} -\mathcal{L}u_n & = & f_n & \boldsymbol{x}\in\Omega_n \\ u_n & = & \theta_n & \boldsymbol{x}\in\widetilde{\Omega}_c \\ u_n & = & 0 & \boldsymbol{x}\in\widetilde{\Omega}_i \end{array}\right. \qquad \left\{\begin{array}{rcll} -\Delta u_l & = & f_l & \boldsymbol{x}\in\Omega_l \\ u_l & = & \theta_l & \boldsymbol{x}\in\Gamma_c \\ u_l & = & 0 & \boldsymbol{x}\in\Gamma_i. \end{array}\right.$$

THE ALGORITHM

Optimization problem:

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

$$\text{s.t.} \quad \left\{ \begin{array}{rcll} -\mathcal{L} u_n & = & f_n & \boldsymbol{x} \in \Omega_n \\ u_n & = & \theta_n & \boldsymbol{x} \in \widetilde{\Omega}_c \\ u_n & = & 0 & \boldsymbol{x} \in \widetilde{\Omega}_i \end{array} \right. \qquad \left\{ \begin{array}{rcll} -\Delta u_l & = & f_l & \boldsymbol{x} \in \Omega_l \\ u_l & = & \theta_l & \boldsymbol{x} \in \Gamma_c \\ u_l & = & 0 & \boldsymbol{x} \in \Gamma_i. \end{array} \right.$$

weak form + finite elements

(using the nonlocal vector calculus)

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

weak form + finite elements

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

THE ALGORITHM

discretized control variables: θ_{nh} and θ_{lh}

A gradient–based algorithm

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

1. **solve the state** equations and compute J_h
2. **compute the gradient** of the functional and evaluate it $\left.\dfrac{\mathrm{d}J_h}{\mathrm{d}(\theta_{nh}, \theta_{lh})}\right|_{(\theta_{nh}^k, \theta_{lh}^k)}$
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 $\theta_{lh}^{k+1} = \theta_{lh}^k + \delta(\theta_{lh}^k)$.

THE ALGORITHM

discretized control variables: θ_{nh} and θ_{lh}

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 and compute J_h $\rightarrow$ **independently!**
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

discretized control variables: θ_{nh} and θ_{lh}

A gradient–based algorithm

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

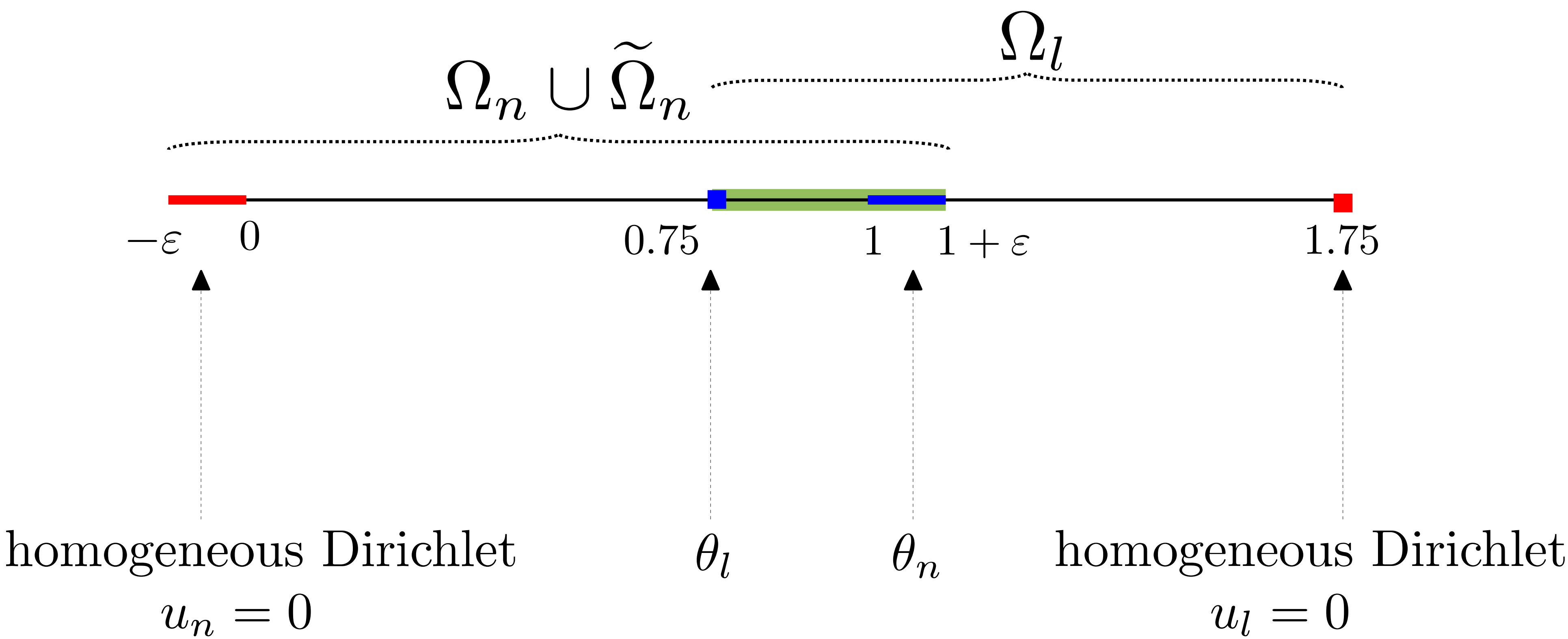
1. **solve the state** equations and compute J_h $\rightarrow$ **independently!**
2. **compute the gradient** of the functional and evaluate it $\left.\dfrac{\mathrm{d}J_h}{\mathrm{d}(\theta_{nh}, \theta_{lh})}\right|_{(\theta^k_{nh}, \theta^k_{lh})}$
3. Use 1. and 2. to **compute the increments** $\delta(\theta^k_{nh})$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

PROBLEM SETTING (1D)



NUMERICAL TESTS

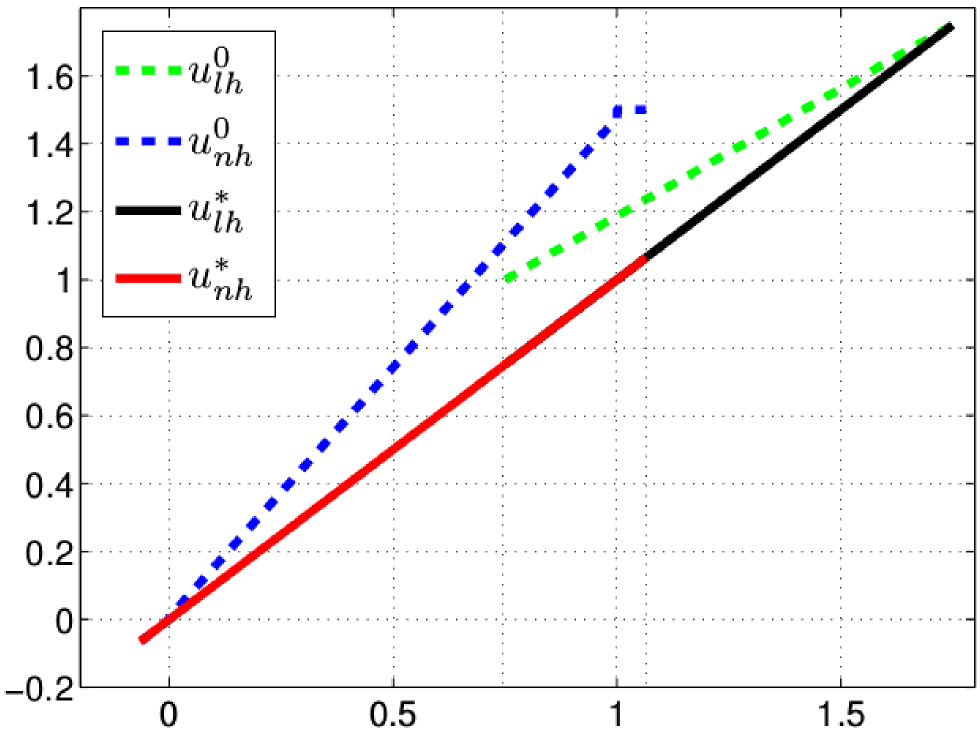
Kernel: $\gamma(x,y) = \dfrac{1}{\varepsilon^2|x-y|}\chi(x-\varepsilon, x+\varepsilon)$

NUMERICAL TESTS

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

The patch test:

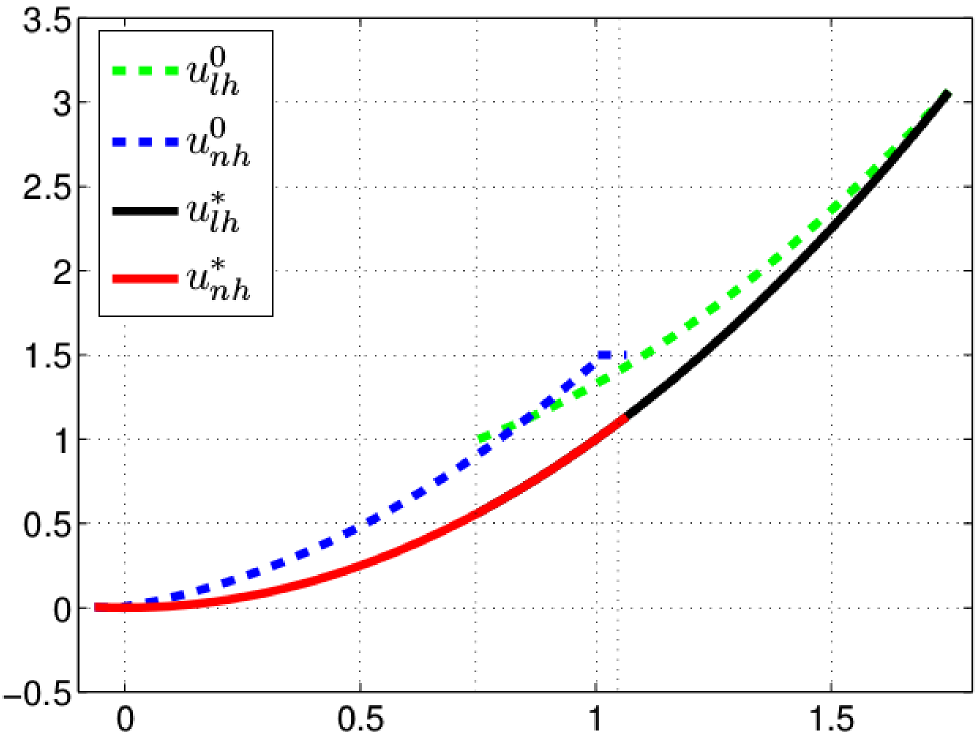
- $u_n = u_l = x$
- $u_n|_{\widetilde{\Omega}_i} = x$
- $u_l(1.75) = 1.75$
- $f_n = f_l = 0$



NUMERICAL TESTS

Accuracy tests:

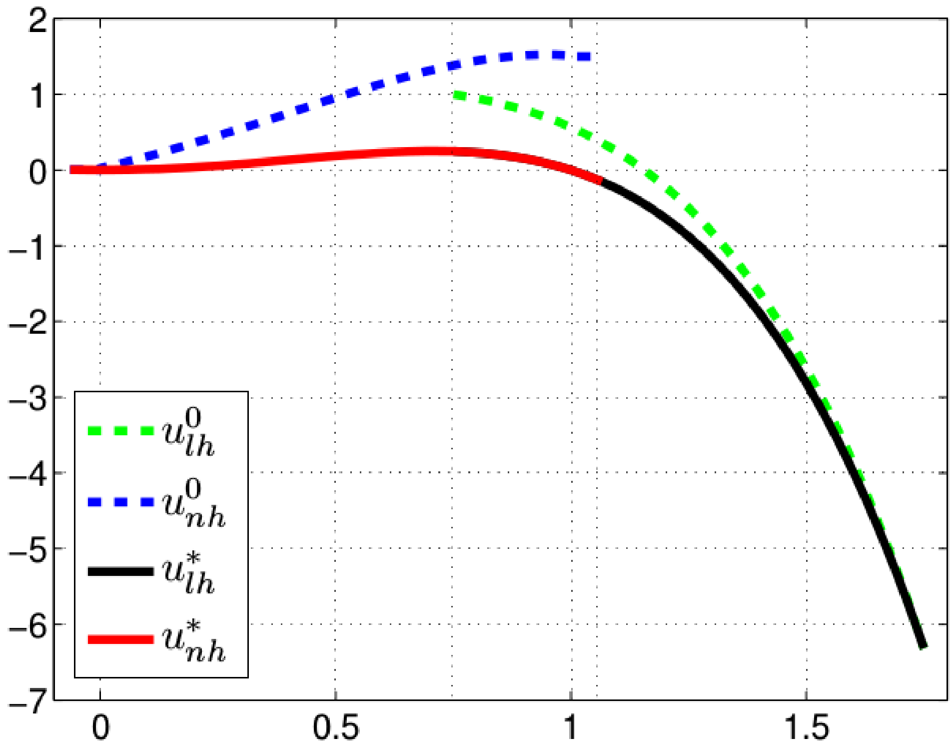
1. - $u_n = u_l = x^2$
   - $u_n|_{\widetilde{\Omega}_i} = x^2$
   - $u_l(1.75) = 1.75^2$
   - $f_n = f_l = -2$



NUMERICAL TESTS

Accuracy tests:

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



NUMERICAL TESTS

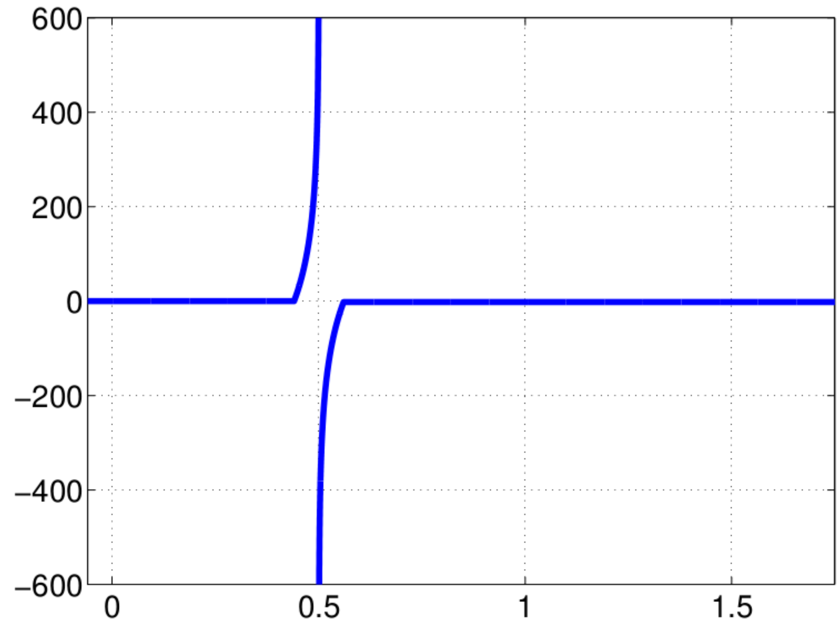
Accuracy tests:

	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:

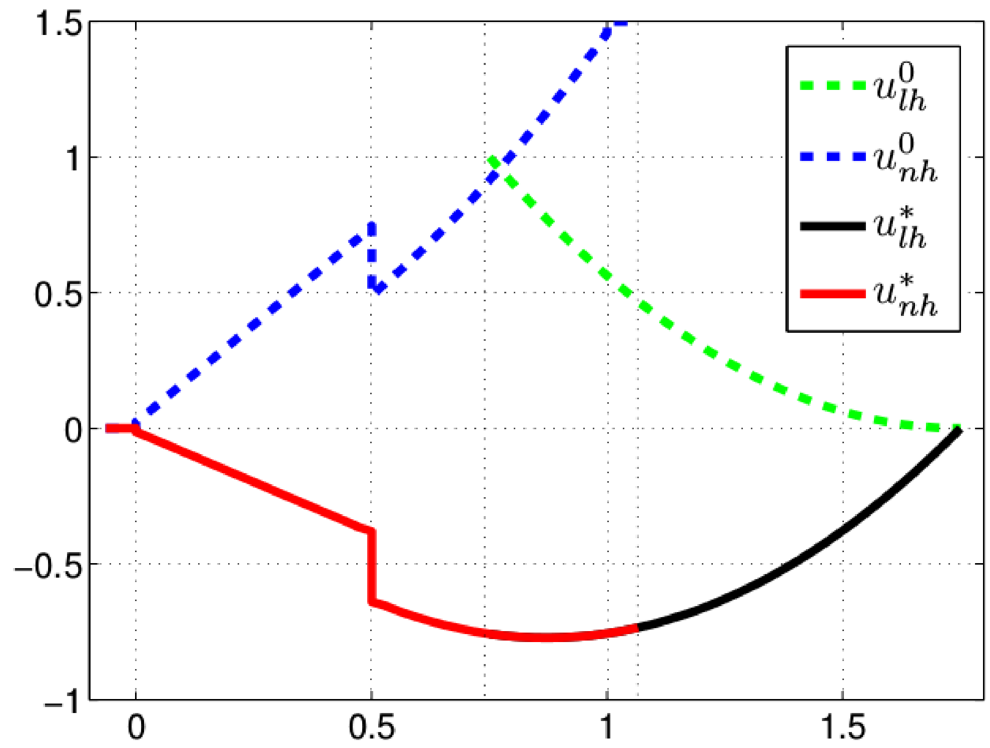
3. • $u_n|_{\widetilde{\Omega}_i} = 0$
   • $u_l(1.75) = 0$



NUMERICAL TESTS

More tests:

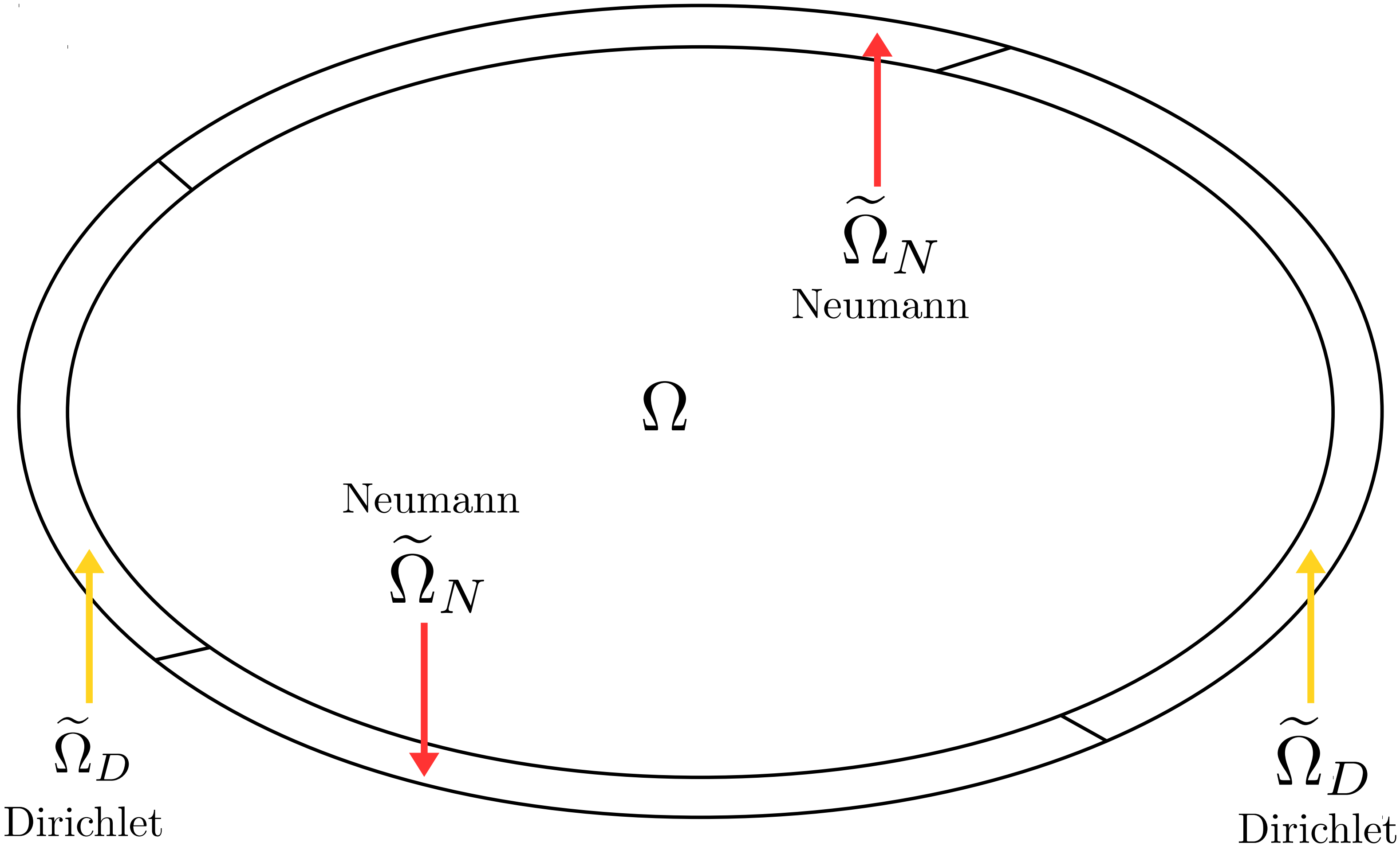
3. • $u_n|_{\widetilde{\Omega}_i} = 0$
   • $u_l(1.75) = 0$



CURRENT WORK

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

MIXED BOUNDARY/VOLUME VALUE PROBLEM



Thank you