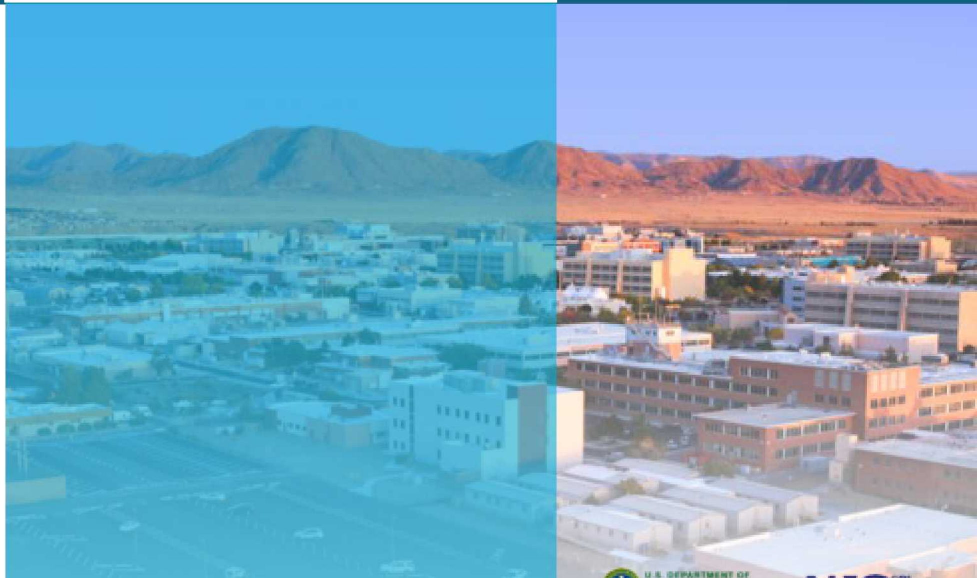
Sandia National Laboratories

SAND2019-9704C

MATNIP – MAThematical foundations for Nonlocal Interface Problems: multiscale simulations for heterogeneous materials

MultiMat 2019



PRESENTED BY

M. D'Elia, *joint work with P. Bochev, G. Capodaglio*, M. Gunzburger*

September 12th 2019

MATNIP LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT

U.S. DEPARTMENT OF ENERGY NNSA

Presentation outline

- **What** is a nonlocal model and **Why** we need an interface theory
- Derivation of a **nonlocal interface theory**
    - Well-posedness
    - Consistency and asymptotic behavior
- Numerical tests
- Next steps

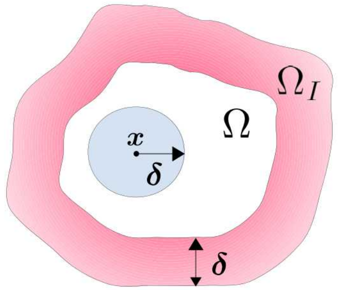
WHAT is a nonlocal model?

WHY do we need an interface theory?

Nonlocal models capture effects that PDEs fail to describe

Basic concepts:

- The state of a system at any point depends on the state in a **neighborhood** of points
- Interactions can occur at distance, without contact
- Solutions can be irregular: non-differentiable, singular, discontinuous



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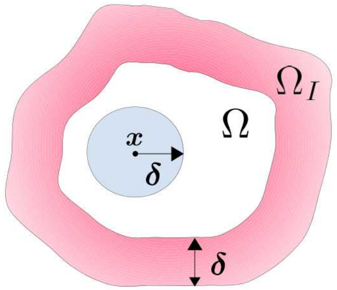
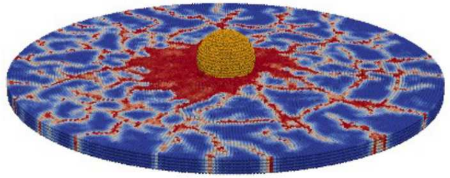


Fact: these models can capture effects that traditional PDEs **fail to capture**

1. Multiscale behaviors & Discontinuities such as cracks and fractures

   e.g. peridynamic model for mechanics



1. Percentage of damage in nonlocal contact mechanics. Littlewood, SNL

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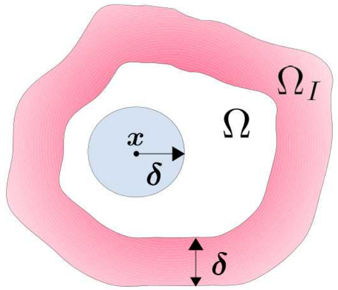

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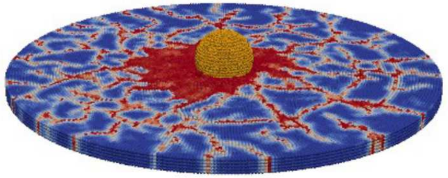
2. Anomalous behaviors such as superdiffusion and subdiffusion

   e.g. fractional differential equations



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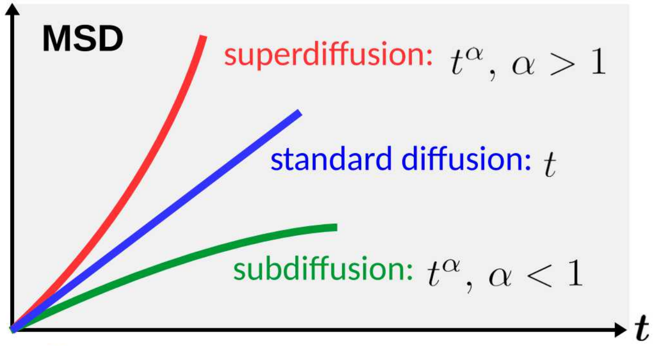

2. **M**ean **S**quare **D**isplacement vs time: broader spectrum of diffusion processes

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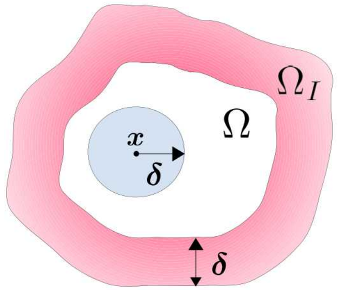

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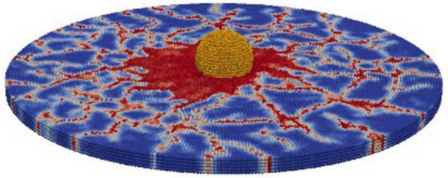

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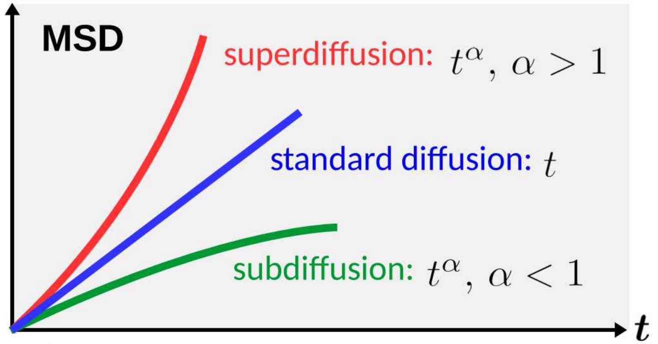

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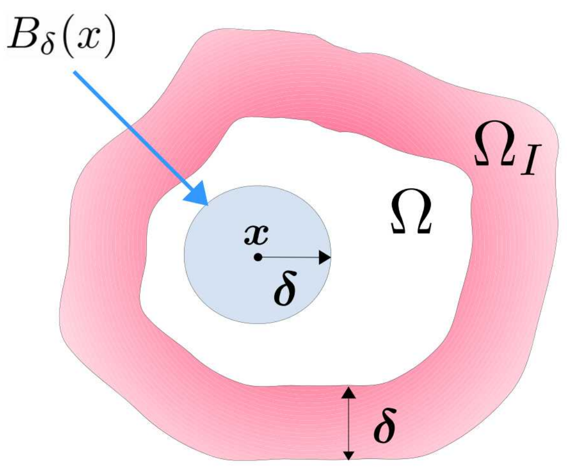
Fact: nonlocal models provide an improved **predictive capability** for

- fracture mechanics
- subsurface flow
- plasma
- stochastic jump processes
- image deblurring/segmentation
- heat conduction

Nonlocal models in one formula



Nonlocal operators (simplest setting)

$Lu(x) = \int_{B_\delta(x)} (u(x) - u(y))k(x,y)dy$, where

- **integral form**: catch long-range forces and reduce regularity requirements
- $Lu \to \Delta u$ as $\delta \to 0$: **convergence to classical diffusion** for vanishing nonlocality
- $k(x,y)$: application dependent kernel

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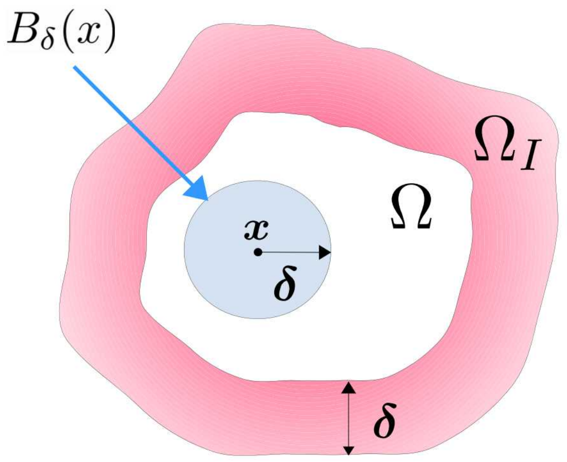

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Nonlocal diffusion

$-Lu = f \quad x \in \Omega$

$+$ conditions on Ω_I

DIFFERENT FROM PDEs!

"Nonlocal boundary conditions" are **prescribed on a layer** surrounding the domain → **volume constraints**

Challenges and goals

Modeling challenges

- prescription of nonlocal boundary conditions
- unknown model parameters
- treatment of nonlocal interfaces

Numerical challenges

- discretizations and their implementation
- design of efficient scalable solvers

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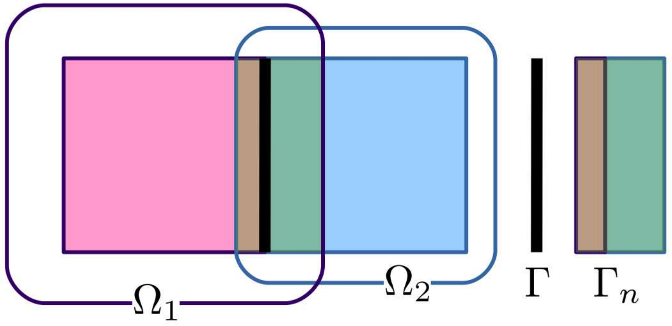
lack of a rigorous nonlocal interface theory, required for

- handling of material discontinuities → physical interfaces
- design of domain-decomposition solvers for efficient simulations → virtual interfaces



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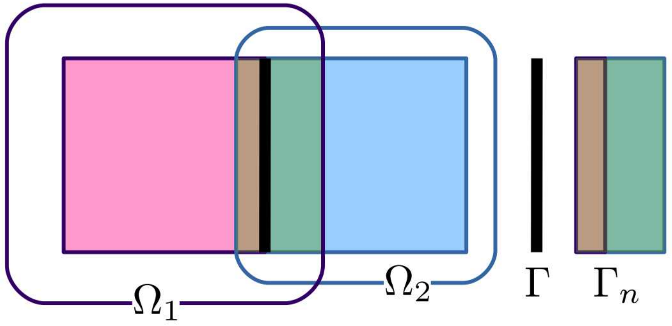
Our goal:

development of a **mathematically rigorous and physically consistent** theory s.t.

- Nonlocal transmission conditions yield **well-posed** interface problems
- Nonlocal interface problems **recover classical formulations** in the local limit



How are interfaces treated right now?

- **Theory:** existing mathematical approaches **fail** to establish rigorous theoretical foundations
  → loss of uniqueness
  → loss of consistency at the local limit

- **Simulations:** several discretizations/implementations are **ad hoc and heuristic**
  → spurious modes, oscillations, mass loss, numerical convergence deterioration

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Novelty of our work

- We derive the nonlocal interface formulation from **energy principles**
- We enforce convergence to local limits
- We ensure existence of a unique solution

A nonlocal interface theory

A Nonlocal Vector Calculus

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

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

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

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

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

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The nonlocal operator L is a composition of divergence and gradient → use **variational theory**

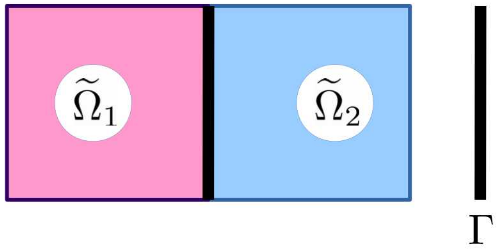
Inspired by Local Interface Problems (LIP)

LIP formulation derived from **energy principles**

Energy minimization

$$\min E_l = \frac{1}{2}\int_{\widetilde{\Omega}_1} \kappa_1 (\nabla u_1)^2 dx + \frac{1}{2}\int_{\widetilde{\Omega}_2} \kappa_2 (\nabla u_2)^2 dx - \int_{\widetilde{\Omega}_1} f_1 u_1 dx - \int_{\widetilde{\Omega}_2} f_2 u_2 dx$$

with $(u_1, u_2) \in H^1(\widetilde{\Omega}_1) \times H^1(\widetilde{\Omega}_2)$



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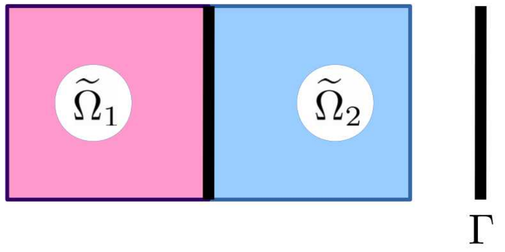

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Optimality conditions

$$-\nabla(\kappa_1 \nabla u_1) = f_1,\ x \in \widetilde{\Omega}_1$$

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$$u_1 = u_2 \quad x \in \Gamma$$ **modeling choice**

$$\kappa_1 \nabla u_1 \cdot \mathbf{n}_1 = \kappa_2 \nabla u_2 \cdot \mathbf{n}_2 \quad x \in \Gamma$$ **outcome of the optimization**

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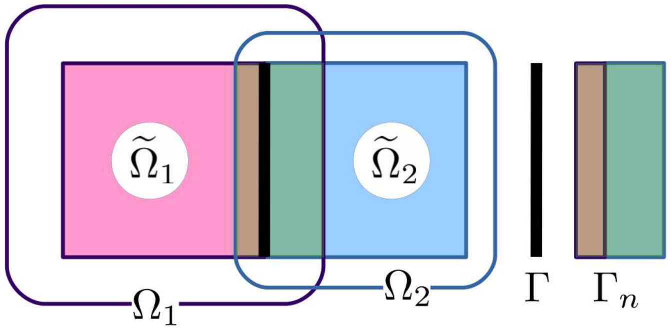

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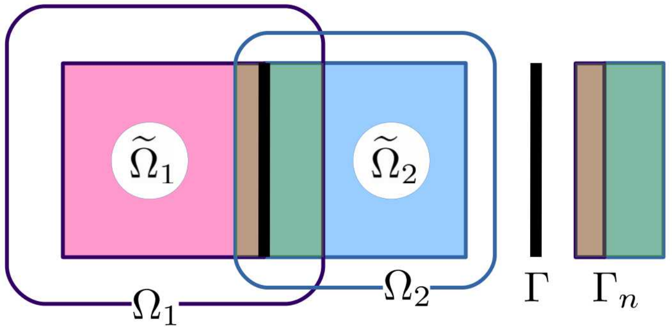

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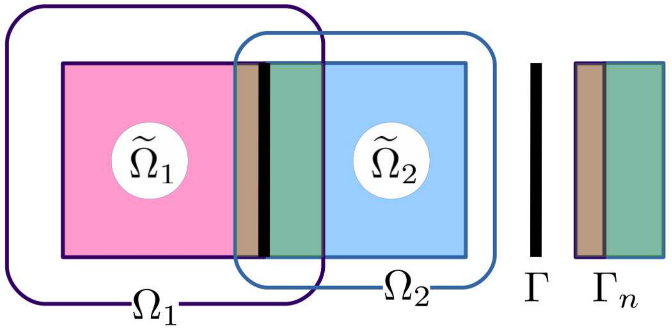

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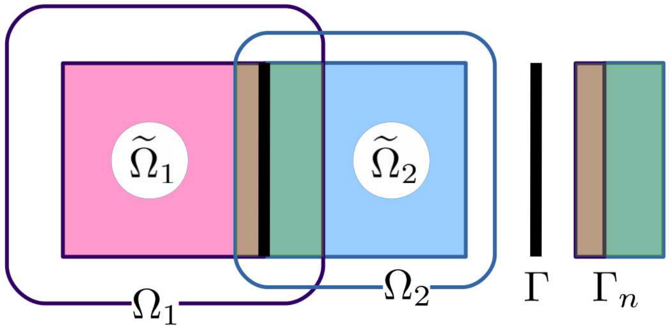

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$\boxed{k_1 \nabla u_1 \cdot \mathbf{n}_1 = k_2 \nabla u_2 \cdot \mathbf{n}_2}$ **local flux condition**

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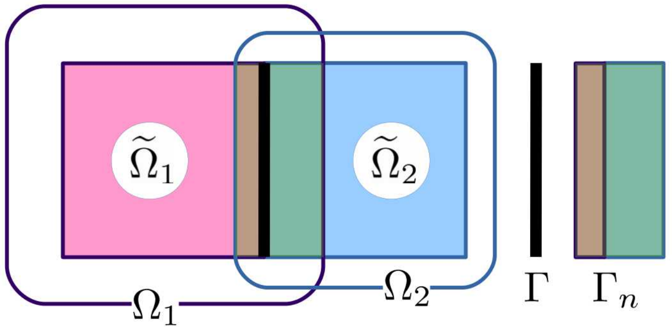

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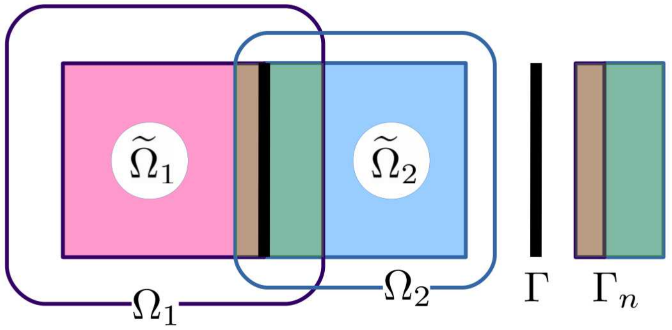

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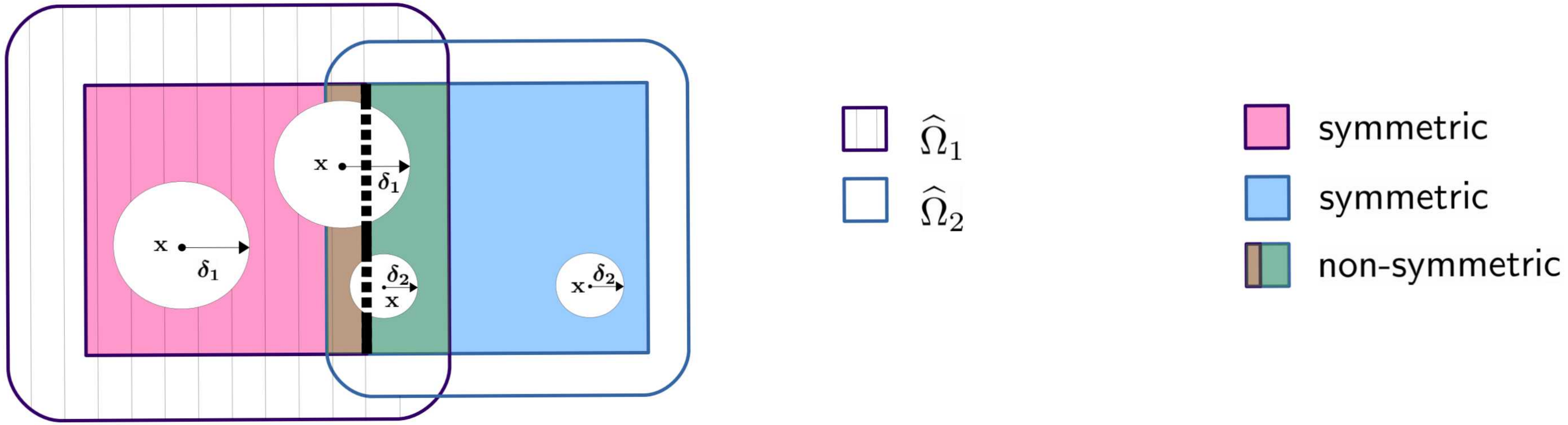
What is the KEY?

definition of the
kernel function
<u>across the interface</u>

How to define the kernel across the interface

A piecewise definition of the kernel function:

$$k(\mathbf{x},\mathbf{y}) = \begin{cases} k_{11}(\mathbf{x},\mathbf{y}) := C(\delta_1)\,\phi_{11}(\mathbf{x},\mathbf{y})\,\mathcal{X}_{B_{\delta_1}(\mathbf{x})}(\mathbf{y}) & \mathbf{x}\in\widehat{\Omega}_1, \mathbf{y}\in\widehat{\Omega}_1 \\ k_{12}(\mathbf{x},\mathbf{y}) := C(\delta_1)\,\phi_{12}(\mathbf{x},\mathbf{y})\,\mathcal{X}_{B_{\delta_1}(\mathbf{x})}(\mathbf{y}) & \mathbf{x}\in\widehat{\Omega}_1, \mathbf{y}\in\widehat{\Omega}_2 \\ k_{21}(\mathbf{x},\mathbf{y}) := C(\delta_2)\,\phi_{21}(\mathbf{x},\mathbf{y})\,\mathcal{X}_{B_{\delta_2}(\mathbf{x})}(\mathbf{y}) & \mathbf{x}\in\widehat{\Omega}_2, \mathbf{y}\in\widehat{\Omega}_1 \\ k_{22}(\mathbf{x},\mathbf{y}) := C(\delta_2)\,\phi_{22}(\mathbf{x},\mathbf{y})\,\mathcal{X}_{B_{\delta_2}(\mathbf{x})}(\mathbf{y}) & \mathbf{x}\in\widehat{\Omega}_2, \mathbf{y}\in\widehat{\Omega}_2, \end{cases}$$



How to define the kernel across the interface

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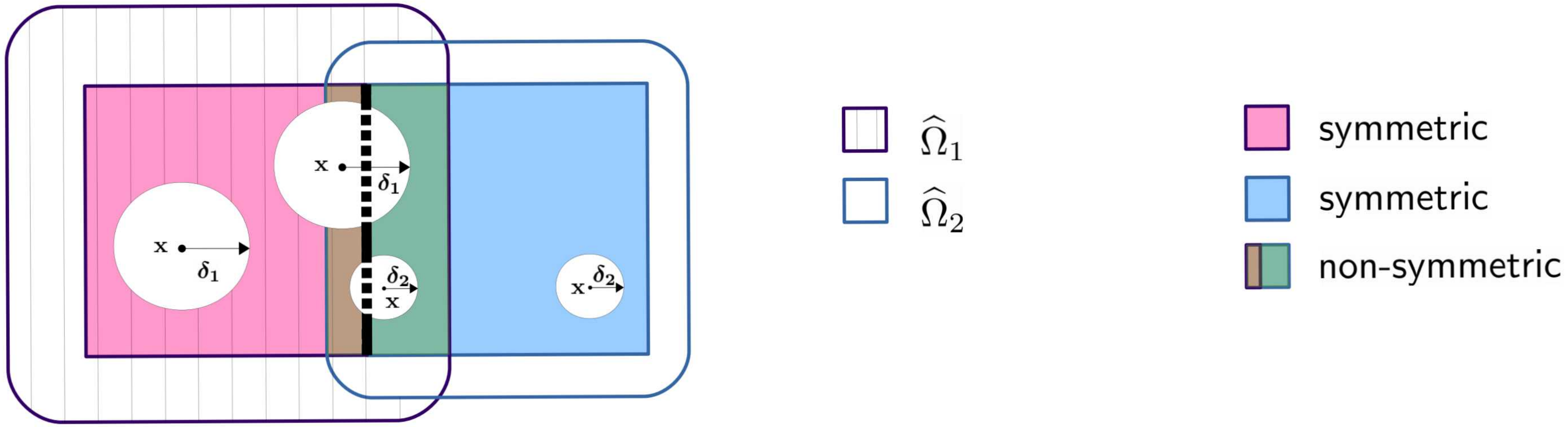
how do we define ϕ?



How to define ϕ

$$k(\mathbf{x},\mathbf{y}) = \begin{cases} k_{11}(\mathbf{x},\mathbf{y}) := C(\delta_1)\, \phi_{11}(\mathbf{x},\mathbf{y})\, \mathcal{X}_{B_{\delta_1}(\mathbf{x})}(\mathbf{y}) & \mathbf{x}\in\widehat{\Omega}_1, \mathbf{y}\in\widehat{\Omega}_1 \\ k_{12}(\mathbf{x},\mathbf{y}) := C(\delta_1)\, \phi_{12}(\mathbf{x},\mathbf{y})\, \mathcal{X}_{B_{\delta_1}(\mathbf{x})}(\mathbf{y}) & \mathbf{x}\in\widehat{\Omega}_1, \mathbf{y}\in\widehat{\Omega}_2 \\ k_{21}(\mathbf{x},\mathbf{y}) := C(\delta_2)\, \phi_{21}(\mathbf{x},\mathbf{y})\, \mathcal{X}_{B_{\delta_2}(\mathbf{x})}(\mathbf{y}) & \mathbf{x}\in\widehat{\Omega}_2, \mathbf{y}\in\widehat{\Omega}_1 \\ k_{22}(\mathbf{x},\mathbf{y}) := C(\delta_2)\, \phi_{22}(\mathbf{x},\mathbf{y})\, \mathcal{X}_{B_{\delta_2}(\mathbf{x})}(\mathbf{y}) & \mathbf{x}\in\widehat{\Omega}_2, \mathbf{y}\in\widehat{\Omega}_2, \end{cases}$$

definition of ϕ_{ii}

kernel functions ϕ_{ii} must be such that **as $\boldsymbol{\delta} \longrightarrow \mathbf{0}$**

$$\begin{array}{lcll} -L_1 u_1 = f_1 & \longrightarrow & -\nabla(\kappa_1 \nabla u_1) = f_1 & x\in\Omega_1 \\ -L_2 u_2 = f_2 & \longrightarrow & -\nabla(\kappa_2 \nabla u_2) = f_2 & x\in\Omega_2 \end{array}$$

the nonlocal equations in the separate domains **converge to the local equations** for $\boldsymbol{\delta} \longrightarrow \mathbf{0}$

How to define ϕ

$$k(\mathbf{x},\mathbf{y}) = \begin{cases} k_{11}(\mathbf{x},\mathbf{y}) := C(\delta_1)\,\phi_{11}(\mathbf{x},\mathbf{y})\,\mathcal{X}_{B_{\delta_1}(\mathbf{x})}(\mathbf{y}) & \mathbf{x}\in\widehat{\Omega}_1, \mathbf{y}\in\widehat{\Omega}_1 \\ k_{12}(\mathbf{x},\mathbf{y}) := C(\delta_1)\,\phi_{12}(\mathbf{x},\mathbf{y})\,\mathcal{X}_{B_{\delta_1}(\mathbf{x})}(\mathbf{y}) & \mathbf{x}\in\widehat{\Omega}_1, \mathbf{y}\in\widehat{\Omega}_2 \\ k_{21}(\mathbf{x},\mathbf{y}) := C(\delta_2)\,\phi_{21}(\mathbf{x},\mathbf{y})\,\mathcal{X}_{B_{\delta_2}(\mathbf{x})}(\mathbf{y}) & \mathbf{x}\in\widehat{\Omega}_2, \mathbf{y}\in\widehat{\Omega}_1 \\ k_{22}(\mathbf{x},\mathbf{y}) := C(\delta_2)\,\phi_{22}(\mathbf{x},\mathbf{y})\,\mathcal{X}_{B_{\delta_2}(\mathbf{x})}(\mathbf{y}) & \mathbf{x}\in\widehat{\Omega}_2, \mathbf{y}\in\widehat{\Omega}_2, \end{cases}$$

definition of ϕ_{ii}

kernel functions ϕ_{ii} must be such that **as $\boldsymbol{\delta \longrightarrow 0}$**

$$-L_1 u_1 = f_1 \quad \longrightarrow \quad -\nabla(\kappa_1 \nabla u_1) = f_1 \quad x\in\Omega_1$$
$$-L_2 u_2 = f_2 \quad \longrightarrow \quad -\nabla(\kappa_2 \nabla u_2) = f_2 \quad x\in\Omega_2$$

the nonlocal equations in the separate domains **converge to the local equations** for $\boldsymbol{\delta \longrightarrow 0}$

condition: $\lim_{\delta_i\to 0} 2\int_{\Omega_i} k_{ii}(\mathbf{x},\mathbf{y})(u_i(\mathbf{x}) - u_i(\mathbf{y}))\,d\mathbf{y} = -\kappa_i \Delta u_i$

2D example*: $C(\delta_i) = \dfrac{4}{\pi\delta_i^4},\ \phi_{ii}(\mathbf{x},\mathbf{y}) = \kappa_i$

next step: determine ϕ_{ij}

*with Euclidean neighborhoods

How to define ϕ

$$k(\mathbf{x},\mathbf{y}) = \begin{cases} k_{11}(\mathbf{x},\mathbf{y}) := C(\delta_1)\,\phi_{11}(\mathbf{x},\mathbf{y})\,\mathcal{X}_{B_{\delta_1}(\mathbf{x})}(\mathbf{y}) & \mathbf{x}\in\widehat{\Omega}_1, \mathbf{y}\in\widehat{\Omega}_1 \\ k_{12}(\mathbf{x},\mathbf{y}) := C(\delta_1)\,\phi_{12}(\mathbf{x},\mathbf{y})\,\mathcal{X}_{B_{\delta_1}(\mathbf{x})}(\mathbf{y}) & \mathbf{x}\in\widehat{\Omega}_1, \mathbf{y}\in\widehat{\Omega}_2 \\ k_{21}(\mathbf{x},\mathbf{y}) := C(\delta_2)\,\phi_{21}(\mathbf{x},\mathbf{y})\,\mathcal{X}_{B_{\delta_2}(\mathbf{x})}(\mathbf{y}) & \mathbf{x}\in\widehat{\Omega}_2, \mathbf{y}\in\widehat{\Omega}_1 \\ k_{22}(\mathbf{x},\mathbf{y}) := C(\delta_2)\,\phi_{22}(\mathbf{x},\mathbf{y})\,\mathcal{X}_{B_{\delta_2}(\mathbf{x})}(\mathbf{y}) & \mathbf{x}\in\widehat{\Omega}_2, \mathbf{y}\in\widehat{\Omega}_2, \end{cases}$$

identification of ϕ_{ij}

1. compute limits of the flux conditions

$$N_1(u_1) - N_2(u_2) = N_*(u_1,u_2) + f \quad \mathbf{x}\in\Gamma_n$$

2. determine kernel parameters such that the limit is

$$\kappa_1\nabla u_1\cdot\mathbf{n}_1 = \kappa_2\nabla u_2\cdot\mathbf{n}_2 \quad \mathbf{x}\in\Gamma$$

How to define ϕ

identification of ϕ_{ij}

1. compute limits of the flux conditions, $\mathbf{x} \in \Omega_1$

$$\frac{4}{\pi\,\delta_1^4}\int_{\Gamma_n\cap B_{\delta_1}(\mathbf{x})} 2\,(u_1(\mathbf{x})-u_1(\mathbf{y}))\,\phi_{11}(\mathbf{x},\mathbf{y})\,d\mathbf{y}$$
$$+\frac{4}{\pi\,\delta_1^4}\int_{\Gamma_n\cap B_{\delta_1}(\mathbf{x})} (u_1(\mathbf{x})-u_2(\mathbf{y}))\,\phi_{12}(\mathbf{x},\mathbf{y})\,d\mathbf{y}$$
$$+\frac{4}{\pi\,\delta_2^4}\int_{\Gamma_n\cap B_{\delta_2}(\mathbf{x})} (u_1(\mathbf{x})-u_2(\mathbf{y}))\,\phi_{21}(\mathbf{y},\mathbf{x})\,d\mathbf{y} = f_1$$

How to define ϕ

identification of ϕ_{ij}

1. compute limits of the flux conditions, $\mathbf{x} \in \Omega_1$

$$
\frac{4}{\pi\,\delta_1^4}\int_{\Gamma_n \cap B_{\delta_1}(\mathbf{x})} 2\,(u_1(\mathbf{x}) - u_1(\mathbf{y}))\,\phi_{11}(\mathbf{x},\mathbf{y})\,d\mathbf{y}
$$
$$
+\frac{4}{\pi\,\delta_1^4}\int_{\Gamma_n \cap B_{\delta_1}(\mathbf{x})} (u_1(\mathbf{x}) - u_2(\mathbf{y}))\,\phi_{12}(\mathbf{x},\mathbf{y})\,d\mathbf{y}
$$
$$
+\frac{4}{\pi\,\delta_2^4}\int_{\Gamma_n \cap B_{\delta_2}(\mathbf{x})} (u_1(\mathbf{x}) - u_2(\mathbf{y}))\,\phi_{21}(\mathbf{y},\mathbf{x})\,d\mathbf{y} = f_1
$$

$\delta \to 0$

$$
\kappa_1 \nabla u_1 \cdot \mathbf{n}_1 = \kappa_2 \nabla u_2 \cdot \mathbf{n}_2 \quad \mathbf{x} \in \Gamma
$$

How to define ϕ

identification of ϕ_{ij}

1. compute limits of the flux conditions, $\mathbf{x} \in \Omega_1$

$$
\begin{aligned}
&\frac{4}{\pi\,\delta_1^4}\int_{\Gamma_n \cap B_{\delta_1}(\mathbf{x})} 2\,(u_1(\mathbf{x}) - u_1(\mathbf{y}))\,\phi_{11}(\mathbf{x},\mathbf{y})\,d\mathbf{y} \\
+&\frac{4}{\pi\,\delta_1^4}\int_{\Gamma_n \cap B_{\delta_1}(\mathbf{x})} (u_1(\mathbf{x}) - u_2(\mathbf{y}))\,\phi_{12}(\mathbf{x},\mathbf{y})\,d\mathbf{y} \\
+&\frac{4}{\pi\,\delta_2^4}\int_{\Gamma_n \cap B_{\delta_2}(\mathbf{x})} (u_1(\mathbf{x}) - u_2(\mathbf{y}))\,\phi_{21}(\mathbf{y},\mathbf{x})\,d\mathbf{y} = f_1
\end{aligned}
$$

Taylor expansion

$$
\begin{aligned}
&\frac{4}{\pi\,\delta_1^4}\Big(-4\big(\mathbf{n}\cdot\nabla u_1(\mathbf{x})\big)\int_0^{\delta_1}\rho^2\phi_{11}(\rho)d\rho \\
&+(\delta_1^2)\int_0^{\delta_1}\rho\phi_{11}(\rho)d\rho + 2\big(\mathbf{n}\cdot\nabla u_2(\mathbf{x})\big)\int_0^{\delta_1}\rho^2\,\phi_{12}(\rho)d\rho \\
&+\Big((\delta_1^2) + (u_1(\mathbf{x}) - u_2(\mathbf{x}))\Big)\int_0^{\delta_1}\rho\phi_{12}(\rho)d\rho\Big) \\
&+\frac{4}{\pi\,\delta_2^4}\Big(2\big(\mathbf{n}\cdot\nabla u_1(\mathbf{x})\big)\int_0^{\delta_2}\rho^2\,\phi_{21}(\rho)d\rho \\
&+(\delta_2^2)\int_0^{\delta_2}\rho\phi_{21}(\rho)d\rho\Big) = f_1
\end{aligned}
$$

?

$\delta \rightarrow 0$

$$\kappa_1 \nabla u_1 \cdot \mathbf{n}_1 = \kappa_2 \nabla u_2 \cdot \mathbf{n}_2 \quad \mathbf{x} \in \Gamma$$

How to define ϕ

identification of ϕ_{ij}

1. compute limits of the flux conditions, $\mathbf{x} \in \Omega_1$

$$\frac{4}{\pi\,\delta_1^4}\int_{\Gamma_n \cap B_{\delta_1}(\mathbf{x})} 2\,(u_1(\mathbf{x}) - u_1(\mathbf{y}))\,\phi_{11}(\mathbf{x},\mathbf{y})\,d\mathbf{y}$$
$$+\frac{4}{\pi\,\delta_1^4}\int_{\Gamma_n \cap B_{\delta_1}(\mathbf{x})} (u_1(\mathbf{x}) - u_2(\mathbf{y}))\,\phi_{12}(\mathbf{x},\mathbf{y})\,d\mathbf{y}$$
$$+\frac{4}{\pi\,\delta_2^4}\int_{\Gamma_n \cap B_{\delta_2}(\mathbf{x})} (u_1(\mathbf{x}) - u_2(\mathbf{y}))\,\phi_{21}(\mathbf{y},\mathbf{x})\,d\mathbf{y} = f_1$$

Taylor expansion

$$\frac{4}{\pi\,\delta_1^4}\boxed{\Big(-4\Big(\mathbf{n}\cdot\nabla u_1(\mathbf{x})\Big)\int_0^{\delta_1}\rho^2\phi_{11}(\rho)d\rho}$$
$$\cancel{+(\delta_1^2)\int_0^{\delta_1}\rho\phi_{11}(\rho)d\rho} + \boxed{2\Big(\mathbf{n}\cdot\nabla u_2(\mathbf{x})\Big)\int_0^{\delta_1}\rho^2\,\phi_{12}(\rho)d\rho}$$
$$\cancel{+\Big((\delta_1^2) + (u_1(\mathbf{x}) - u_2(\mathbf{x}))\Big)\int_0^{\delta_1}\rho\phi_{12}(\rho)d\rho\Big)}$$
$$+\frac{4}{\pi\,\delta_2^4}\boxed{\Big(2\Big(\mathbf{n}\cdot\nabla u_1(\mathbf{x})\Big)\int_0^{\delta_2}\rho^2\,\phi_{21}(\rho)d\rho}$$
$$\cancel{+(\delta_2^2)\int_0^{\delta_2}\rho\phi_{21}(\rho)d\rho\Big) = f_1}$$

?

$\delta \longrightarrow 0$

$\delta \longrightarrow 0$

$$\kappa_1 \nabla u_1 \cdot \mathbf{n}_1 = \kappa_2 \nabla u_2 \cdot \mathbf{n}_2 \quad \mathbf{x} \in \Gamma$$

How to define ϕ

M.D'Elia

identification of ϕ_{ij}

1. compute limits of the flux conditions, $\mathbf{x} \in \Omega_1$

$$\frac{4}{\pi\,\delta_1^4}\int_{\Gamma_n \cap B_{\delta_1}(\mathbf{x})} 2\,(u_1(\mathbf{x}) - u_1(\mathbf{y}))\,\phi_{11}(\mathbf{x},\mathbf{y})\,d\mathbf{y}$$
$$+\frac{4}{\pi\,\delta_1^4}\int_{\Gamma_n \cap B_{\delta_1}(\mathbf{x})} (u_1(\mathbf{x}) - u_2(\mathbf{y}))\,\phi_{12}(\mathbf{x},\mathbf{y})\,d\mathbf{y}$$
$$+\frac{4}{\pi\,\delta_2^4}\int_{\Gamma_n \cap B_{\delta_2}(\mathbf{x})} (u_1(\mathbf{x}) - u_2(\mathbf{y}))\,\phi_{21}(\mathbf{y},\mathbf{x})\,d\mathbf{y} = f_1$$

Taylor expansion

$$\frac{4}{\pi\,\delta_1^4}\Big(-4\Big(\mathbf{n}\cdot\nabla u_1(\mathbf{x})\Big)\int_0^{\delta_1}\rho^2\phi_{11}(\rho)d\rho$$
$$\cancel{+(\delta_1^2)\int_0^{\delta_1}\rho\phi_{11}(\rho)d\rho} + 2\Big(\mathbf{n}\cdot\nabla u_2(\mathbf{x})\Big)\int_0^{\delta_1}\rho^2\,\phi_{12}(\rho)d\rho$$
$$\cancel{+\Big((\delta_1^2)+(u_1(\mathbf{x})-u_2(\mathbf{x}))\Big)\int_0^{\delta_1}\rho\phi_{12}(\rho)d\rho\Big)}$$
$$+\frac{4}{\pi\,\delta_2^4}\Big(2\Big(\mathbf{n}\cdot\nabla u_1(\mathbf{x})\Big)\int_0^{\delta_2}\rho^2\,\phi_{21}(\rho)d\rho$$
$$\cancel{+(\delta_2^2)\int_0^{\delta_2}\rho\phi_{21}(\rho)d\rho\Big) = f_1}$$

$\delta \rightarrow 0$

$\delta \rightarrow 0$

$$\kappa_1 \nabla u_1 \cdot \mathbf{n}_1 = \kappa_2 \nabla u_2 \cdot \mathbf{n}_2 \quad \mathbf{x} \in \Gamma$$

2. determine kernel parameters

$$\frac{1}{3c}\delta_1^3\,\kappa_2 = \int_0^{\delta_1}\rho^2\phi_{12}(\rho)d\rho \qquad \frac{1}{2c}\delta_1^2\,\kappa_2 = \int_0^{\delta_1}\rho\phi_{12}(\rho)d\rho$$

$$\frac{c}{3}\delta_2^3\,\kappa_1 = \int_0^{\delta_2}\rho^2\phi_{21}(\rho)d\rho \qquad \frac{c}{2}\delta_2^2\,\kappa_1 = \int_0^{\delta_2}\rho\phi_{21}(\rho)d\rho$$

How to define ϕ

M.D'Elia

identification of ϕ_{ij}

1. compute limits of the flux conditions, $\mathbf{x} \in \Omega_1$

$$\frac{4}{\pi\,\delta_1^4}\int_{\Gamma_n \cap B_{\delta_1}(\mathbf{x})} 2\,(u_1(\mathbf{x}) - u_1(\mathbf{y}))\,\phi_{11}(\mathbf{x},\mathbf{y})\,d\mathbf{y}$$
$$+\frac{4}{\pi\,\delta_1^4}\int_{\Gamma_n \cap B_{\delta_1}(\mathbf{x})} (u_1(\mathbf{x}) - u_2(\mathbf{y}))\,\phi_{12}(\mathbf{x},\mathbf{y})\,d\mathbf{y}$$
$$+\frac{4}{\pi\,\delta_2^4}\int_{\Gamma_n \cap B_{\delta_2}(\mathbf{x})} (u_1(\mathbf{x}) - u_2(\mathbf{y}))\,\phi_{21}(\mathbf{y},\mathbf{x})\,d\mathbf{y} = f_1$$

Taylor expansion

$$\frac{4}{\pi\,\delta_1^4}\left(-4\Big(\mathbf{n}\cdot\nabla u_1(\mathbf{x})\Big)\int_0^{\delta_1}\rho^2\phi_{11}(\rho)d\rho\right.$$
$$\cancel{+(\delta_1^2)\int_0^{\delta_1}\rho\phi_{11}(\rho)d\rho} + 2\Big(\mathbf{n}\cdot\nabla u_2(\mathbf{x})\Big)\int_0^{\delta_1}\rho^2\,\phi_{12}(\rho)d\rho$$
$$\cancel{+\Big((\delta_1^2) + (u_1(\mathbf{x}) - u_2(\mathbf{x}))\Big)\int_0^{\delta_1}\rho\phi_{12}(\rho)d\rho\Big)}$$
$$+\frac{4}{\pi\,\delta_2^4}\left(2\Big(\mathbf{n}\cdot\nabla u_1(\mathbf{x})\Big)\int_0^{\delta_2}\rho^2\,\phi_{21}(\rho)d\rho\right.$$
$$\cancel{+(\delta_2^2)\int_0^{\delta_2}\rho\phi_{21}(\rho)d\rho\Big) = f_1}$$

$\delta \to 0$

2. determine kernel parameters

$$\frac{1}{3c}\delta_1^3\,\kappa_2 = \int_0^{\delta_1}\rho^2\phi_{12}(\rho)d\rho \qquad \frac{1}{2c}\delta_1^2\,\kappa_2 = \int_0^{\delta_1}\rho\phi_{12}(\rho)d\rho$$

$$\frac{c}{3}\delta_2^3\,\kappa_1 = \int_0^{\delta_2}\rho^2\phi_{21}(\rho)d\rho \qquad \frac{c}{2}\delta_2^2\,\kappa_1 = \int_0^{\delta_2}\rho\phi_{21}(\rho)d\rho$$

Applying conditions

$$\kappa_1\nabla u_1\cdot\mathbf{n}_1 = \kappa_2\nabla u_2\cdot\mathbf{n}_2 \quad \mathbf{x}\in\Gamma$$

$\delta \to 0$

M.D'Elia

How to define ϕ

identification of ϕ_{ij}

1. compute limits of the flux conditions, $\mathbf{x} \in \Omega_1$

$$
\begin{aligned}
&\frac{4}{\pi\,\delta_1^4}\int_{\Gamma_n \cap B_{\delta_1}(\mathbf{x})} 2\,(u_1(\mathbf{x}) - u_1(\mathbf{y}))\,\phi_{11}(\mathbf{x},\mathbf{y})\,d\mathbf{y} \\
&+\frac{4}{\pi\,\delta_1^4}\int_{\Gamma_n \cap B_{\delta_1}(\mathbf{x})} (u_1(\mathbf{x}) - u_2(\mathbf{y}))\,\phi_{12}(\mathbf{x},\mathbf{y})\,d\mathbf{y} \\
&+\frac{4}{\pi\,\delta_2^4}\int_{\Gamma_n \cap B_{\delta_2}(\mathbf{x})} (u_1(\mathbf{x}) - u_2(\mathbf{y}))\,\phi_{21}(\mathbf{y},\mathbf{x})\,d\mathbf{y} = f_1
\end{aligned}
$$

Taylor expansion

$$
\begin{aligned}
&\frac{4}{\pi\,\delta_1^4}\Big(-4\big(\mathbf{n}\cdot\nabla u_1(\mathbf{x})\big)\int_0^{\delta_1}\rho^2\phi_{11}(\rho)d\rho \\
&\cancel{+(\delta_1^2)\int_0^{\delta_1}\rho\phi_{11}(\rho)d\rho} + 2\big(\mathbf{n}\cdot\nabla u_2(\mathbf{x})\big)\int_0^{\delta_1}\rho^2\,\phi_{12}(\rho)d\rho \\
&\cancel{+\Big((\delta_1^2)+(u_1(\mathbf{x})-u_2(\mathbf{x}))\Big)\int_0^{\delta_1}\rho\phi_{12}(\rho)d\rho\Big)} \\
&+\frac{4}{\pi\,\delta_2^4}\Big(2\big(\mathbf{n}\cdot\nabla u_1(\mathbf{x})\big)\int_0^{\delta_2}\rho^2\,\phi_{21}(\rho)d\rho \\
&\cancel{+(\delta_2^2)\int_0^{\delta_2}\rho\phi_{21}(\rho)d\rho\Big) = f_1}
\end{aligned}
$$

What kernels satisfy these conditions?

$\delta \to 0$

2. determine kernel parameters

$$
\frac{1}{3c}\delta_1^3\,\kappa_2 = \int_0^{\delta_1}\rho^2\phi_{12}(\rho)d\rho \qquad \frac{1}{2c}\delta_1^2\,\kappa_2 = \int_0^{\delta_1}\rho\phi_{12}(\rho)d\rho
$$

$$
\frac{c}{3}\delta_2^3\,\kappa_1 = \int_0^{\delta_2}\rho^2\phi_{21}(\rho)d\rho \qquad \frac{c}{2}\delta_2^2\,\kappa_1 = \int_0^{\delta_2}\rho\phi_{21}(\rho)d\rho
$$

Applying conditions

$$
\kappa_1\nabla u_1\cdot\mathbf{n}_1 = \kappa_2\nabla u_2\cdot\mathbf{n}_2 \quad \mathbf{x}\in\Gamma
$$

How to define ϕ

identification of ϕ_{ij}

1. compute limits of the flux conditions, $\mathbf{x} \in \Omega_1$

$$
\begin{aligned}
&\frac{4}{\pi\,\delta_1^4}\int_{\Gamma_n \cap B_{\delta_1}(\mathbf{x})} 2\,(u_1(\mathbf{x}) - u_1(\mathbf{y}))\,\phi_{11}(\mathbf{x},\mathbf{y})\,d\mathbf{y} \\
+&\frac{4}{\pi\,\delta_1^4}\int_{\Gamma_n \cap B_{\delta_1}(\mathbf{x})} (u_1(\mathbf{x}) - u_2(\mathbf{y}))\,\phi_{12}(\mathbf{x},\mathbf{y})\,d\mathbf{y} \\
+&\frac{4}{\pi\,\delta_2^4}\int_{\Gamma_n \cap B_{\delta_2}(\mathbf{x})} (u_1(\mathbf{x}) - u_2(\mathbf{y}))\,\phi_{21}(\mathbf{y},\mathbf{x})\,d\mathbf{y} = f_1
\end{aligned}
$$

Taylor expansion

$$
\begin{aligned}
&\frac{4}{\pi\,\delta_1^4}\boxed{\Big(-4\big(\mathbf{n}\cdot\nabla u_1(\mathbf{x})\big)\int_0^{\delta_1}\rho^2\phi_{11}(\rho)d\rho} \\
&\cancel{+(\delta_1^2)\int_0^{\delta_1}\rho\phi_{11}(\rho)d\rho} + \boxed{2\big(\mathbf{n}\cdot\nabla u_2(\mathbf{x})\big)\int_0^{\delta_1}\rho^2\,\phi_{12}(\rho)d\rho} \\
&\cancel{+\Big((\delta_1^2) + (u_1(\mathbf{x}) - u_2(\mathbf{x}))\Big)\int_0^{\delta_1}\rho\phi_{12}(\rho)d\rho\Big)} \\
&+\frac{4}{\pi\,\delta_2^4}\boxed{\Big(2\big(\mathbf{n}\cdot\nabla u_1(\mathbf{x})\big)\int_0^{\delta_2}\rho^2\,\phi_{21}(\rho)d\rho} \\
&\cancel{+(\delta_2^2)\int_0^{\delta_2}\rho\phi_{21}(\rho)d\rho\Big) = f_1}
\end{aligned}
$$

What kernels satisfy these conditions?

$\delta \to 0$

$$\kappa_1 \nabla u_1 \cdot \mathbf{n}_1 = \kappa_2 \nabla u_2 \cdot \mathbf{n}_2 \quad \mathbf{x} \in \Gamma$$

Applying conditions

2. determine kernel parameters

2D example:

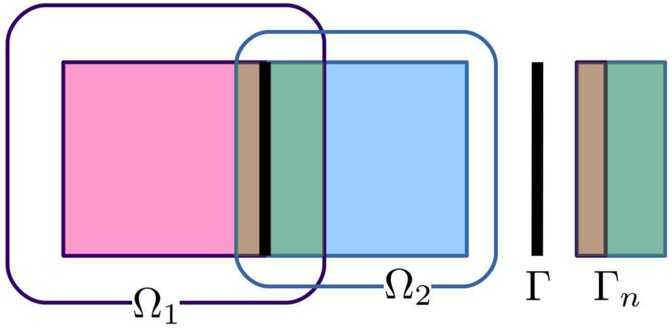
$$\phi_{12}(\mathbf{x},\mathbf{y}) = \frac{\kappa_2}{c},\; \phi_{21}(\mathbf{x}, yb) = \kappa_1$$

Well-posedness of NIP

Equivalent formulation

$$E_n = \frac{1}{2}\iint_{\widehat{\Omega}_1} (Gu_1)^2 k(x,y)dydx + \frac{1}{2}\iint_{\widehat{\Omega}_2} (Gu_2)^2 k(x,y)dydx - \int_{\widetilde{\Omega}_1} f_1 u_1 dx - \int_{\widetilde{\Omega}_2} f_2 u_2 dx$$

$$E_n = \frac{1}{2}\iint_{\Omega_1\cup\Omega_2} (Gu)^2 k(x,y)dydx - \int_{\widetilde{\Omega}_1\cup\widetilde{\Omega}_2} f u dx$$

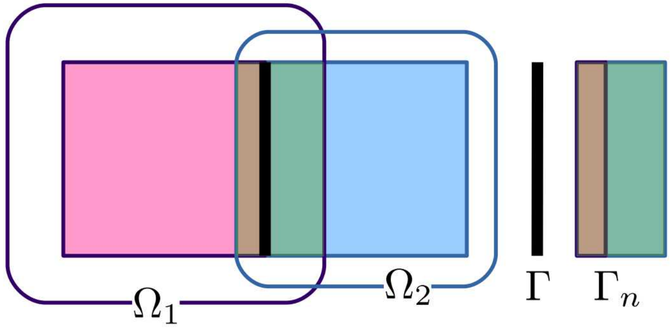


Well-posedness of NIP

Equivalent formulation

$$E_n = \frac{1}{2}\iint_{\widehat{\Omega}_1} (Gu_1)^2 k(x,y)\,dy dx + \frac{1}{2}\iint_{\widehat{\Omega}_2} (Gu_2)^2 k(x,y)\,dy dx - \int_{\widetilde{\Omega}_1} f_1 u_1 dx - \int_{\widetilde{\Omega}_2} f_2 u_2 dx$$

$$E_n = \frac{1}{2}\iint_{\Omega_1\cup\Omega_2} (Gu)^2 k(x,y)\,dy dx - \int_{\widetilde{\Omega}_1\cup\widetilde{\Omega}_2} f u\, dx$$



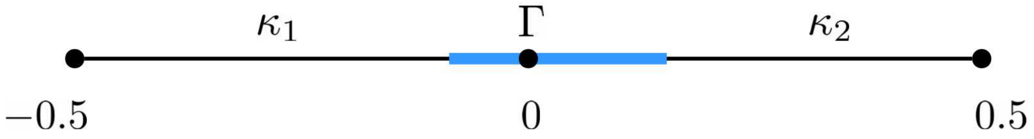
Euler-Lagrange equations

$$\underbrace{\iint_{\Omega_1\cup\Omega_2} (Gu)(Gv) k(x,y)\,dy dx}_{} = \int_{\widetilde{\Omega}_1\cup\widetilde{\Omega}_2} f v\, dx \quad \forall\, v \in V$$

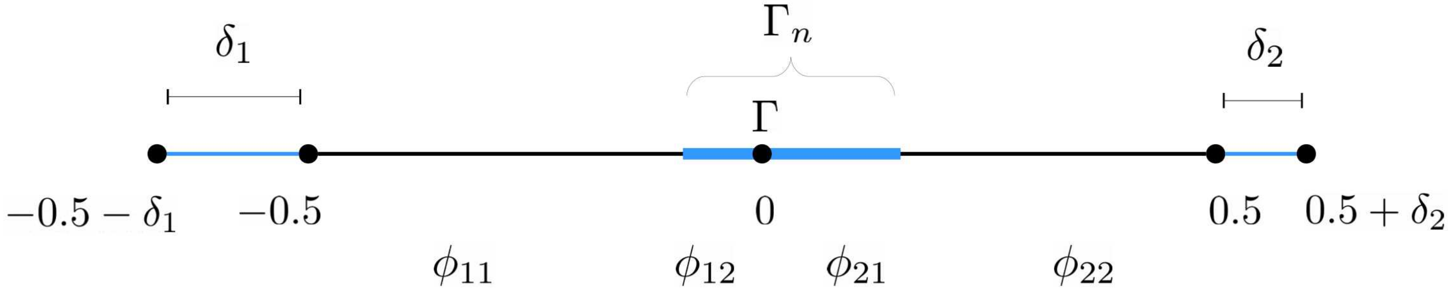
coercive form → well-posedness

Numerical tests

1D test case: problem setting



local domain



nonlocal domain

$$k(x,y) = \begin{cases} k_{11}(x,y) := \dfrac{2}{3\delta_1^3}\, \phi_{11}(x,y)\, \mathcal{X}_{B_{\delta_1}(x)}(y) & x < 0.5, y < 0.5 \\ k_{12}(x,y) := \dfrac{2}{3\delta_1^3}\, \phi_{12}(x,y)\, \mathcal{X}_{B_{\delta_1}(x)}(y) & x < 0.5, y > 0.5 \\ k_{21}(x,y) := \dfrac{2}{3\delta_2^3}\, \phi_{21}(x,y)\, \mathcal{X}_{B_{\delta_2}(x)}(y) & x > 0.5, y < 0.5 \\ k_{22}(x,y) := \dfrac{2}{3\delta_2^3}\, \phi_{22}(x,y)\, \mathcal{X}_{B_{\delta_2}(x)}(y) & x > 0.5, y > 0.5 \end{cases}$$

$$\phi_{ii}(x,y) = \kappa_i$$

$$\phi_{12}(x,y) = \frac{\kappa_*}{**}$$

$$\phi_{21}(x,y) = \frac{\kappa_*}{**}$$

1D test case: optimal h-convergence

Problem parameters

$f_1(x) = f_2(x) = 1,$

$g_1(x) = \frac{1}{16} - \frac{1}{8}x - \frac{1}{2}x^2$, $g_2(x) = \frac{1}{16} - \frac{1}{24}x - \frac{1}{6}x^2$

$\delta_1 = 2^{-5}$, $\delta_2 = 2^{-4}$, $\kappa_1 = 1$, $\kappa_2 = 3$

Reference solution & error

u_{ref}: reference solution on a grid of size $h_{ref} = 2^{-13}$

error: $e = \|u - u_{ref}\|_{L^2(\Omega_1 \cup \Omega_2)}$

h	e	order
2^{-5}	5.274e-5	-
2^{-6}	1.310e-5	2.009
2^{-7}	3.159e-6	2.051
2^{-8}	7.610e-7	2.053
2^{-9}	1.879e-7	2.017

h	interface gap
2^{-5}	6.497e-4
2^{-6}	4.227e-4
2^{-7}	4.169e-4
2^{-8}	4.151e-4
2^{-9}	4.148e-4

1D test case: optimal h-convergence

Problem parameters

$f_1(x) = f_2(x) = 1,$

$g_1(x) = \frac{1}{16} - \frac{1}{8}x - \frac{1}{2}x^2,\; g_2(x) = \frac{1}{16} - \frac{1}{24}x - \frac{1}{6}x^2$

$\delta_1 = 2^{-5},\; \delta_2 = 2^{-4},\; \kappa_1 = 1,\; \kappa_2 = 3$

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stagnation: the gap is part of the solution!

1D test case: δ-convergence

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$h = 2^{-11}$

Local solution & error

u_L: analytic local solution for $\kappa_1 = 1,\ \kappa_2 = 3$

error: $e_L = \|u - u_L\|_{L^2(\Omega_1 \cup \Omega_2)}$

δ_1	δ_2	e_L	order
2^{-4}	2^{-3}	4.701e-4	-
2^{-5}	2^{-4}	1.623e-4	1.534
2^{-6}	2^{-5}	6.692e-5	1.277
2^{-7}	2^{-6}	3.109e-5	1.106
2^{-8}	2^{-7}	1.516e-5	1.035
2^{-9}	2^{-8}	7.520e-6	1.011
2^{-10}	2^{-9}	3.763e-6	0.999

δ_1	δ_2	e_L	order
2^{-4}	2^{-3}	6.854e-4	-
2^{-5}	2^{-4}	4.147e-4	0.725
2^{-6}	2^{-5}	2.249e-4	0.883
2^{-7}	2^{-6}	1.167e-4	0.946
2^{-8}	2^{-7}	5.950e-5	0.972
2^{-9}	2^{-8}	3.000e-5	0.988
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1D test case: δ-convergence

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the gap converges to $\mathbf{0}$

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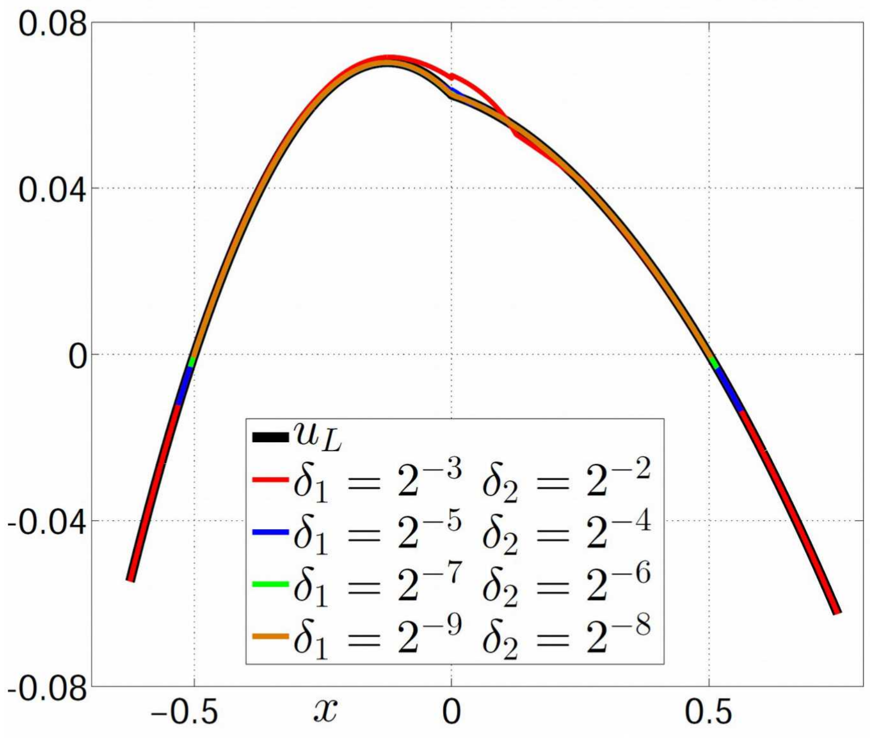

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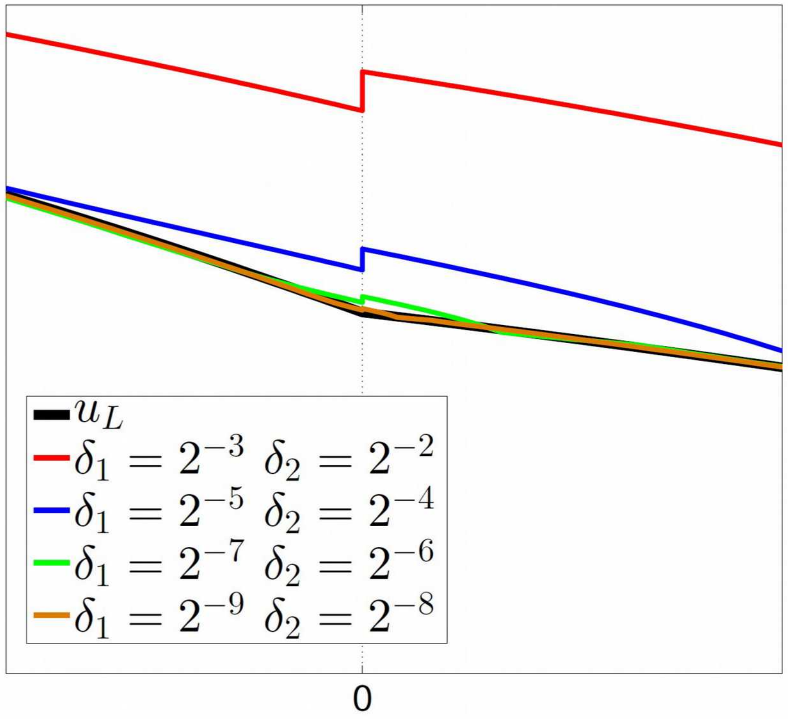
the gap converges to **0**



Future work

Our plan

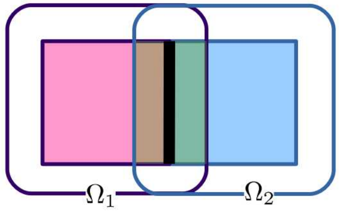
Nonlocal interface theory

Virtual interfaces

Nonlocal Domain Decomposition

Two-domain

Multi-domain



Fractional capability

Advection capability

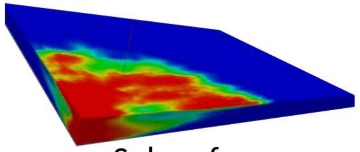
Physical interfaces

Applications

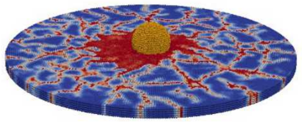
Subsurface diffusion

Subsurface transport

Mechanics



Subsurface CO_2 dispersion

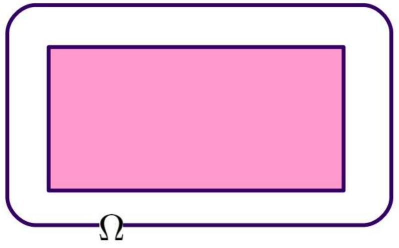


Damage mechanics

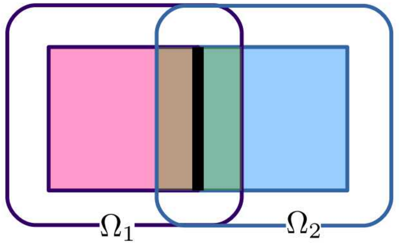
Domain Decomposition for fast computations

Fact: the numerical solution of NLM can be **prohibitively expensive**

Proposed approach: mimic local DD technique FETI and certify its validity with MATNIP



creation of virtual interfaces by domain decomposition



enabling parallel solvers $\longrightarrow$ speed-up

first scalable DD solvers and preconditioners

Local FETI: solution of the saddle-point problem

$$\mathbb{L}(v_1, v_2, \mu) = E_l(v_1, v_2) + \int_\Gamma (v_1 - v_2)\mu$$

equivalent to (LIP)! $\rightarrow$ (LIP) used to certify properties of FETI

nFETI: solution of the **nonlocal** saddle-point problem

$$\mathbb{L}(v_1, v_2, \mu) = E_n(v_1, v_2) + \int_{\Gamma_n} (v_1 - v_2)\mu$$

equivalent to (NIP)?? $\rightarrow$ (NIP) is a fundamental tool for nonlocal DD

Outcome: nFETI could **drastically increase the usability** of NLMs, currently hindered by prohibitive costs

QUESTIONS?

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