Coupling of Multi-fidelity Models
Applications to PNP-cDFT and local-nonlocal Poisson equations

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CM4 summer school, Stanford, June 21st

Center for Computing Research

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Outline

- Why we need to couple different models
- Brief introduction of classic Schwarz methods
- PNP and cDFT equations for electrostatics
- Some facts about nonlocal models
- Coupling PNP-cDFT with Schwarz
- Optimization-based coupling
- Nonlocal Poisson equation as a proxy for Peridynamics
- Coupling of local and nonlocal Poisson equations

Hands-on sessions (with Kyungjoo Kim):

- Schwarz and Optimization-based couplings of local and nonlocal Poisson equations

Why we need coupling techniques

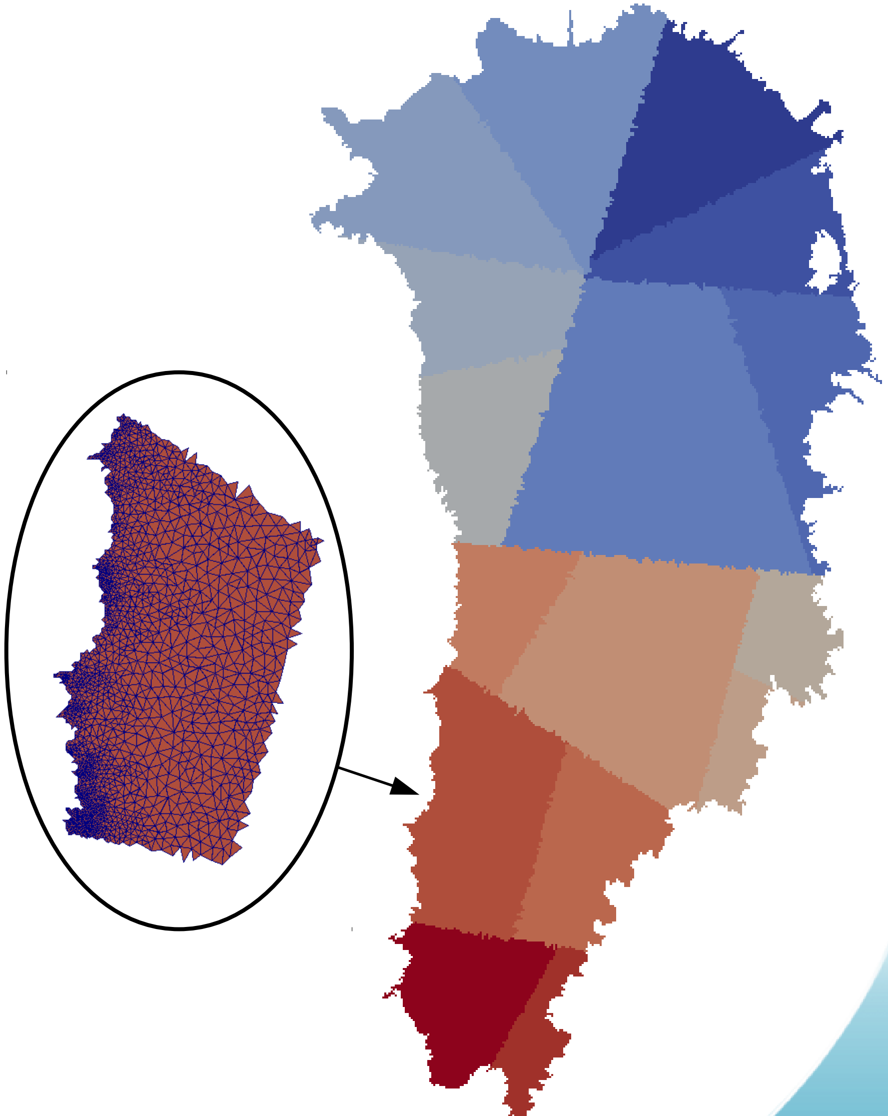
Example1: Domain Decomposition (same model, multiple domains)

- Problem restricted to each subdomain is smaller and requires less resources (memory and CPU).

- Iterative parallel solution: problem on subdomains can be solved independently and then at each iteration values at the interfaces are “communicated” to neighbor domains.

- Problem can be solved in parallel over multiple processes.

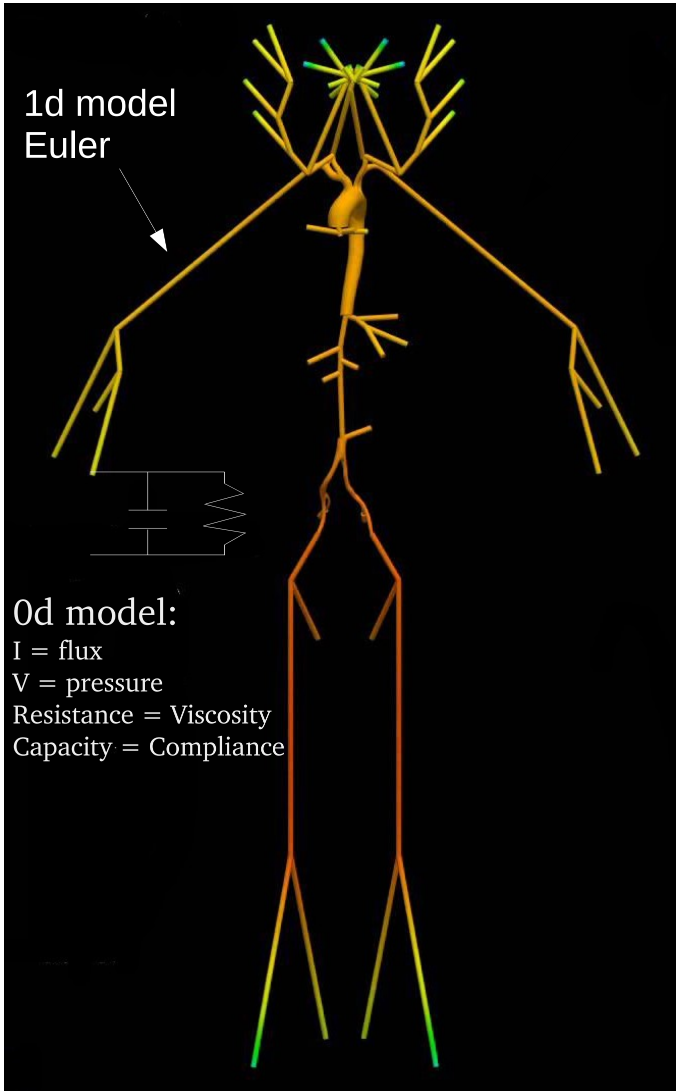
- Domain Decomposition methods are often used to create preconditioners for iterative solvers.



Typical interface conditions for Poisson-like problems:
1. Continuity of solution
2. Continuity of solution derivative normal to the surface

Why we need coupling techniques

Example2: Modeling systemic circulation (geometric multiscale*)

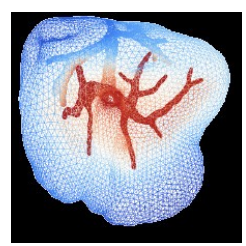


Simulations by Cristiano Malossi (CMCS), LifeV

Aorta, 3D model:
Navier-Stokes

How to couple NS (aorta)
With 1D Euler (other vessels)?

And what about
Fluid-Structure Interaction?



Liver, 3D model:
Darcy flow

How to couple NS (large vessel)
with Darcy (porous media)?

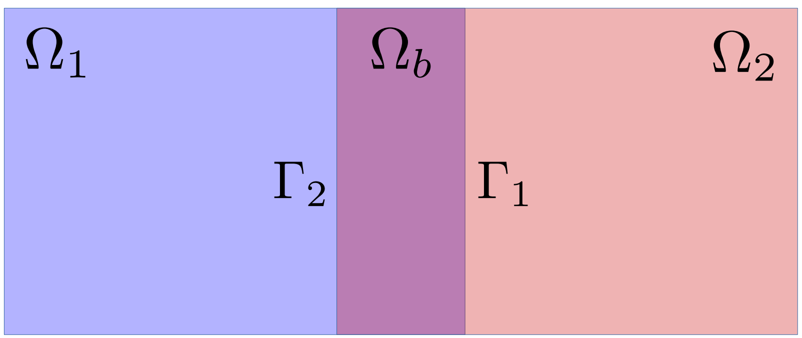
NS: vector equation.
Darcy: scalar equation.

*__Quarteroni, Formaggia, Veneziani__, Cardiovascular mathematics, Springer, 2009

Alternating Schwarz methods

Alternating Schwarz Method

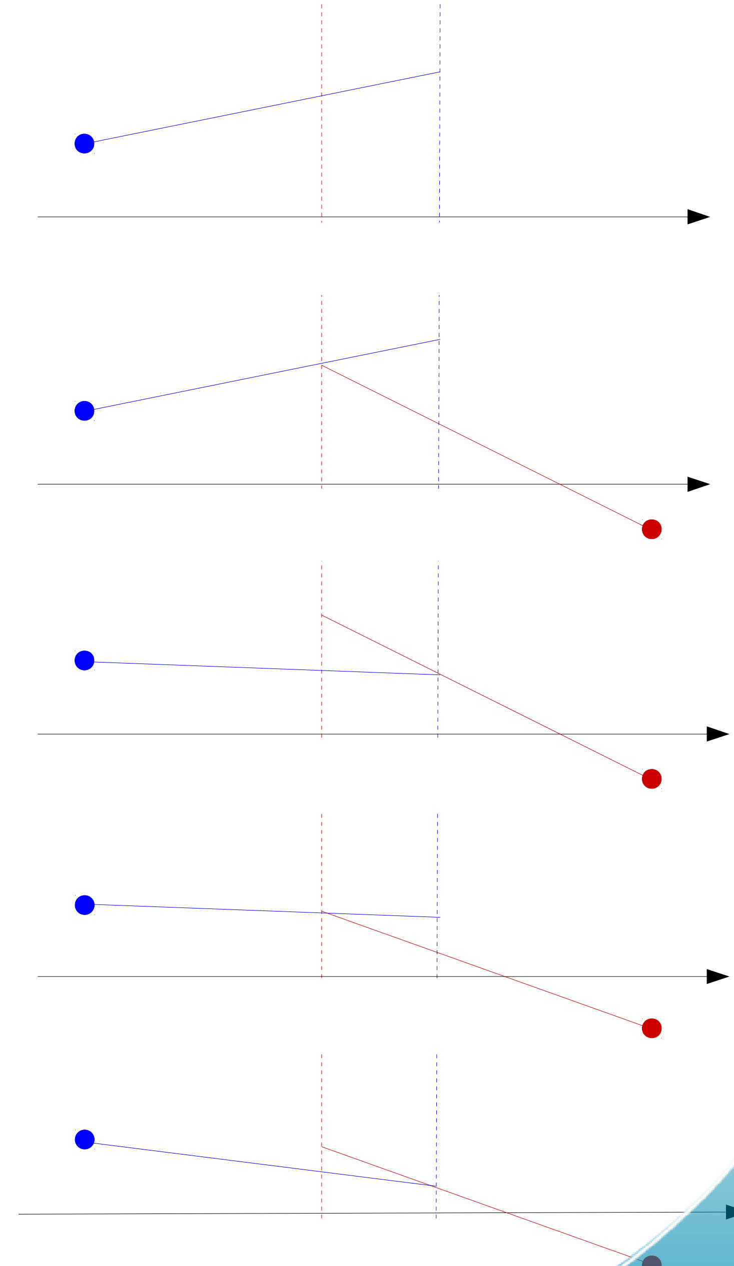
Laplace problem: $\begin{cases} -\Delta u = 0 & \text{in } \Omega \\ \text{proper b.c.} & \text{on } \partial\Omega \end{cases}$



$$\Omega_b := \Omega_1 \cap \Omega_2, \quad \Omega := \Omega_1 \cup \Omega_2$$

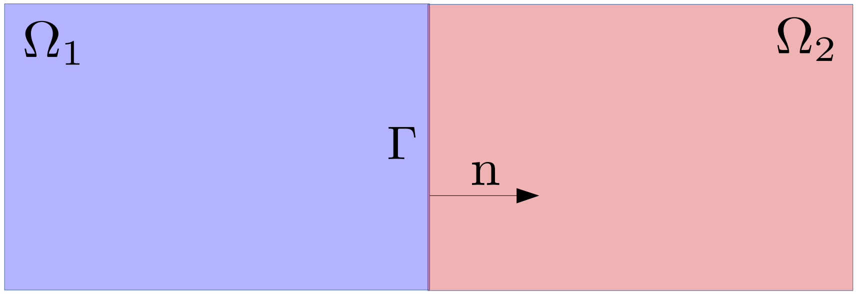
$$\begin{cases} -\Delta u_1^{k+1} = 0 & \text{in } \Omega_1 \\ u_1^{k+1} = u_2^{k} & \text{on } \Gamma_1 \\ \text{other b.c.} \end{cases} \qquad \begin{cases} -\Delta u_2^{k+1} = 0 & \text{in } \Omega_2 \\ u_2^{k+1} = u_1^{k(+1)} & \text{on } \Gamma_2 \\ \text{other b.c.} \end{cases}$$

- Converges with elliptic operators
- Rate of convergence depends on the size of the overlap
- Overlap needed for convergence

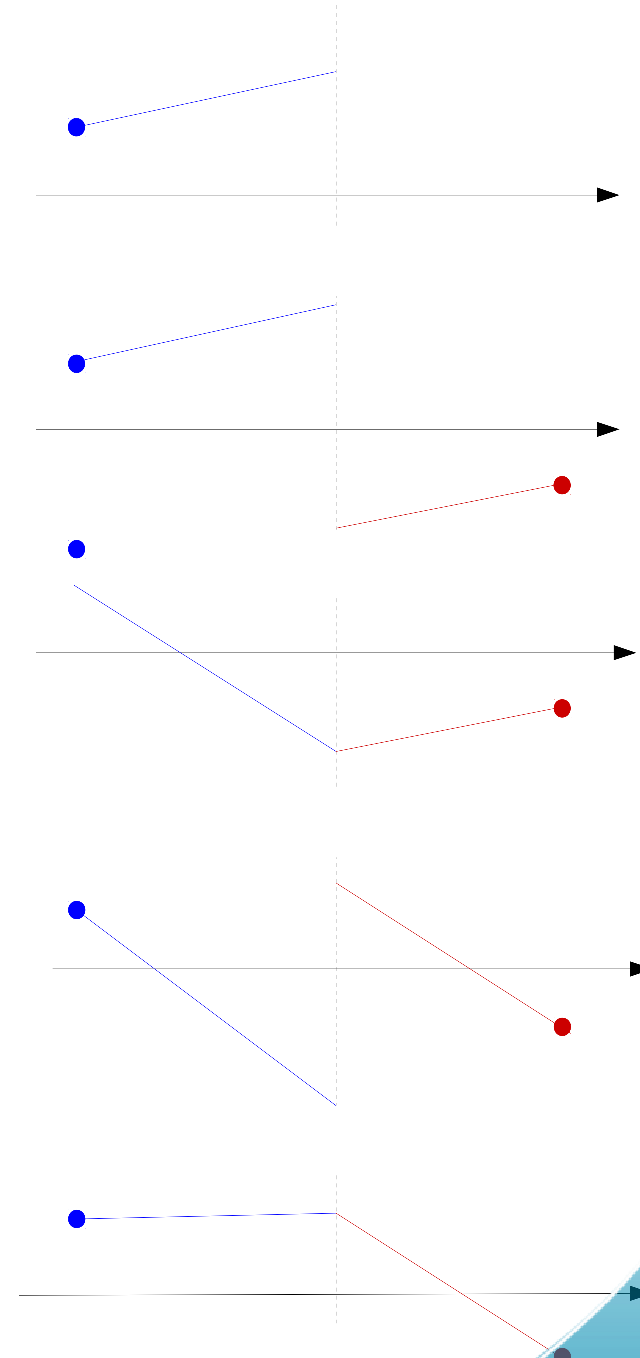


Toselli and Widlund, Domain Decomposition Methods – Algorithms and Theory, Springer, 2005

(Nonoverlapping) Coupling Methods



$$\Gamma := \Omega_1 \cap \Omega_2$$



Dirichlet-Neumann methods

$$\begin{cases} -\Delta u_1^{k+1} = 0 & \text{in } \Omega_1 \\ u_1^{k+1} = u_2^{k} & \text{on } \Gamma_1 \\ \text{other b.c.} & \end{cases} \qquad \begin{cases} -\Delta u_2^{k+1} = 0 & \text{in } \Omega_2 \\ \partial_n u_2^{k+1} = \partial_n u_1^{k+1} & \text{on } \Gamma_2 \\ \text{other b.c.} & \end{cases}$$

Robin-Robin methods

$$\begin{cases} -\Delta u_1^{k+1} = 0 & \text{in } \Omega_1 \\ \alpha_1 u_1^{k+1} + \partial_n u_1^{k+1} = \alpha_1 u_2^{k} + \partial_n u_2^{k+1} & \text{on } \Gamma_1 \\ \text{other b.c.} & \end{cases}$$

$$\begin{cases} -\Delta u_2^{k+1} = 0 & \text{in } \Omega_2 \\ \alpha_2 u_2^{k+1} + \partial_n u_2^{k+1} = \alpha_2 u_1^{k+1} + \partial_n u_1^{k+1} & \text{on } \Gamma_2 \\ \text{other b.c.} & \end{cases}$$

We can select α_1 and α_2 to improve convergence:

- **M. Gander**, Optimized Schwarz Methods, SIAM J. Numer. Anal., 2006

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Poisson-Nerst-Planck and classic Density Functional Theory

Poisson-Nernst-Planck (PNP) equations

Poisson equation for electric potential

$$\text{div}\,(-\epsilon\nabla\phi) = q$$

ϕ : electric potential
q : charge density
ϵ : dielectric constant

Nernst Planck equation for each ion type

$$\frac{\partial\rho_\alpha}{\partial t} + \text{div}(\mathbf{\Phi}_\alpha) = 0$$

$$\mathbf{\Phi}_\alpha := \rho_\alpha\mathbf{v} - D_\alpha\nabla\rho_\alpha - \tfrac{D_\alpha e z_\alpha}{kT}\rho_\alpha\nabla\phi$$

$$q := e\sum_\alpha \rho_\alpha z_\alpha$$

ρ_α : density of ion α
D_α : diffusion constant for ion α
$\mathbf{\Phi}_\alpha$: ion flux
z_α : valence of ion α, values: $\pm 1, \pm 2, \ldots$
T : temperature
e : electron charge
K : Boltzmann gas constant

Boundary and initial conditions:

Poisson: $\phi = \phi^{\text{bd}}$, or $-\epsilon\dfrac{\partial\phi}{\partial n} = q_\sigma^{\text{bd}}$

Nernst-Planck: $\rho_\alpha = \rho_\alpha^{\text{bd}}$, or $\mathbf{\Phi}_\alpha \cdot \mathbf{n} = \Phi_\alpha^{\text{bd}}$

if $\dfrac{\partial\rho_\alpha}{\partial t} = 0 \rightarrow$ steady state PNP
if $\mathbf{\Phi}_\alpha = \mathbf{0}, \quad \mathbf{v} = \mathbf{0} \rightarrow$ Poisson Boltzmann Approx.

Classic Density Functional Theory (cDFT)

Equivalently, the ion flux can be expressed in terms of the chemical potential

$$\boldsymbol{\Phi}_\alpha := \rho_\alpha \mathbf{u} - D_\alpha \nabla \rho_\alpha - \tfrac{D_\alpha e z_\alpha}{kT} \rho_\alpha \nabla \phi = \rho_\alpha \mathbf{u} - D_\alpha \rho_\alpha \nabla \mu_\alpha,$$

$$\mu_\alpha = \ln(\rho_\alpha) + \frac{e z_\alpha}{KT}\phi$$

chemical potential

$$\left(\begin{array}{l} \text{Use formula:} \\ \nabla(\ln(\rho_\alpha)) = \dfrac{1}{\rho_\alpha}\nabla \rho_\alpha \end{array} \right)$$

Add terms to the chemical potential that account for ion correlation and finite size

$$\mu_\alpha^{cDFT} = \ln(\rho_\alpha) + \frac{e z_\alpha}{KT}\phi + \left(V + \frac{\partial F^{\text{ex}}}{\partial \rho_\alpha} \right)$$

V : external chemical potential
F^{ex} : excess Helmholtz free energy

$$F^{\text{ex}}(\rho) = F^{\text{hs}}(\rho) + F^{\text{corr}}(\rho) + F^{\text{disp}}(\rho)$$

F^{hs} : hard-sphere free energy
F^{corr} : second-order charge correlations
F^{disp} : mean-field interactions

The excess Helmholtz free energy terms are **nonlocal** terms:

$$\frac{\partial F^{\text{corr}}}{\partial \rho_\alpha} = -\sum_\beta \int_\Omega \rho_\beta(\mathbf{y}) c_{\alpha\beta}(|\mathbf{x} - \mathbf{y}|) \mathrm{d}\mathbf{y}$$

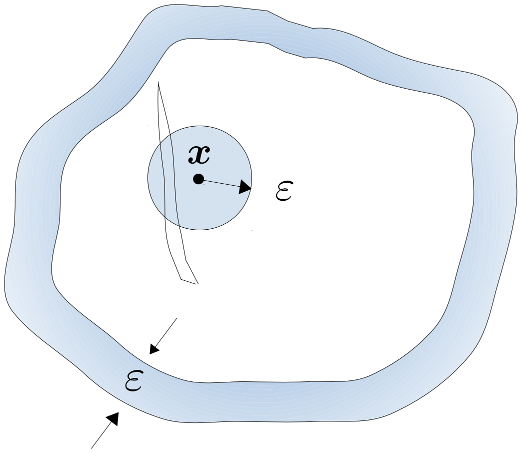
- **R Roth, R Evans, A Lang, and G Kahl.** Fundamental measure theory for hard-sphere mixtures revisited: the white bear version. J Phys-Condens Mat, 2002.

Facts about Nonlocal Models

Facts about Nonlocal Models

- Nonlocal operators $\mathcal{L}(u)(\boldsymbol{x})$ depend on the values of u in a *finite/infinite* neighbour of $\boldsymbol{x}$
- Interactions can occur at distance, without contact
- Boundary conditions need to be prescribed on an ϵ border of the domain
- Used in many scientific and engineering applications, where the material dynamics depends on microstructure, e.g. nonlocal electrostatic or brittle fracture
- Often, under some regularity assumption, as the horizon ε goes to zero, or equivalently as we take a macroscopic look at the model, the nonlocal model reduces to a local model

$$\mathcal{L}(u)(\boldsymbol{x}) = \int_{B(x,\varepsilon)} u(y)c(|x-y|)\mathrm{d}y$$



– **Q. Du, M.D. Gunzburger, R. Lehoucq, and K. Zhou**, Analysis and approximation of nonlocal diffusion problems with volume constraints. *SIAM Review*, 2012

Comparison of Local and Nonlocal discretizations

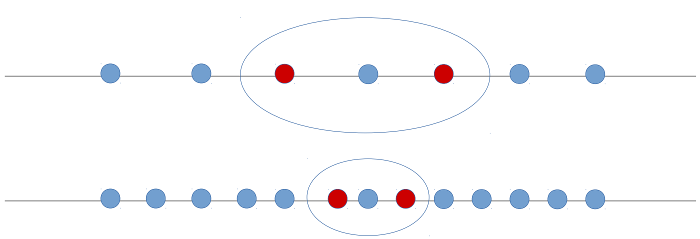
Local operator $\left.\frac{du}{dx}\right|_x$

Depends on the values that u takes in an *infinitesimum* neighbour of $\mathbf{x}$

Simple discretization:

$$\left|\frac{du}{dx}\right|_{x_i} \approx \frac{u(x_{i+1}) - u(x_{i-1})}{x_{i+1} - x_{i-1}}$$

#evaluations: 2 (in one dimension)



#evaluations: $2d$ (in d dimesions, gradient)

Nonzeros of discretization matrices grow **linearly** with the number of points, or as h^{-d}.

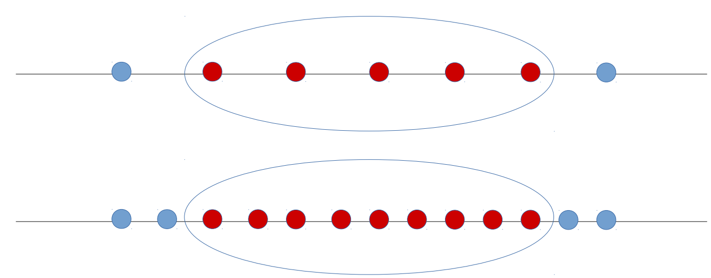
Nonocal operator $\int_{B(x,\varepsilon)} u(y)c(|x-y|)\mathrm{d}y$

Depends on the values that u takes in a *finite/infinite* neighbour of $\mathbf{x}$

Simple discretization:

$$\sum_{|x_j - x_i| < \varepsilon} u(x_j)c(|x_j - x_i|)w_j^h$$

evaluations: $\approx 2\frac{\varepsilon}{h}$ (in one dimension)



evaluations: $\approx V_{\mathcal{B}(0,1)} \frac{\varepsilon^d}{h^d}$ (in d dimensions)

Nonzeros of discretization matrices grow as the **square** of the number of unknowns, or as h^{-2d}.

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PNP-DFT Coupling

Work by J. Cheung, A. Frishknecht, M. Perego, P. Bochev

Comparing PNP and DFT models

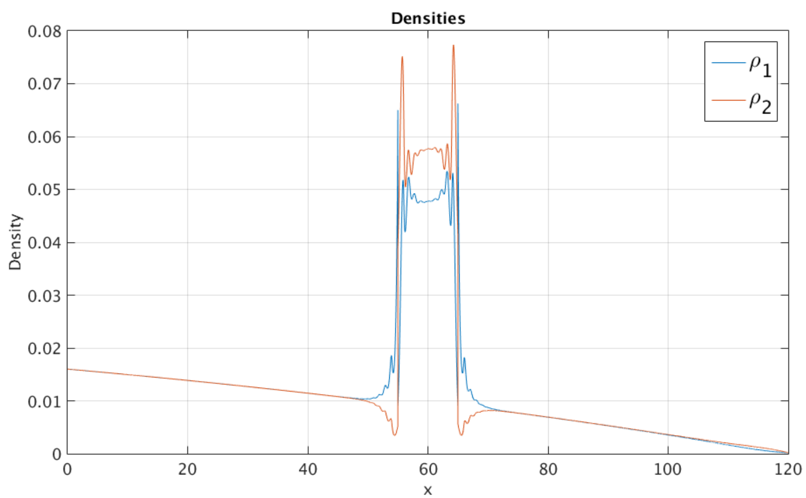
Problem: Semi-permeable membrane

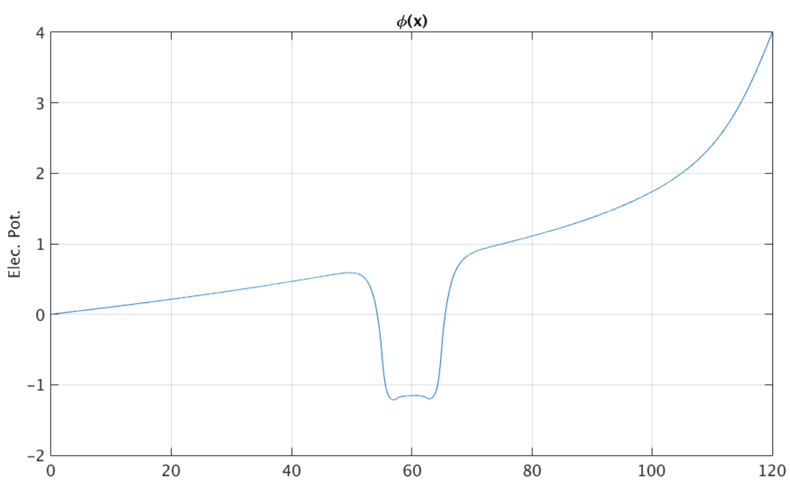
$\rho^{\pm} = 0.016$
$\rho^{0} = 0.7$
$\phi = 0$

$\rho^{\pm} = 0.00016$
$\rho^{0} = 0.7$
$\phi = 4$

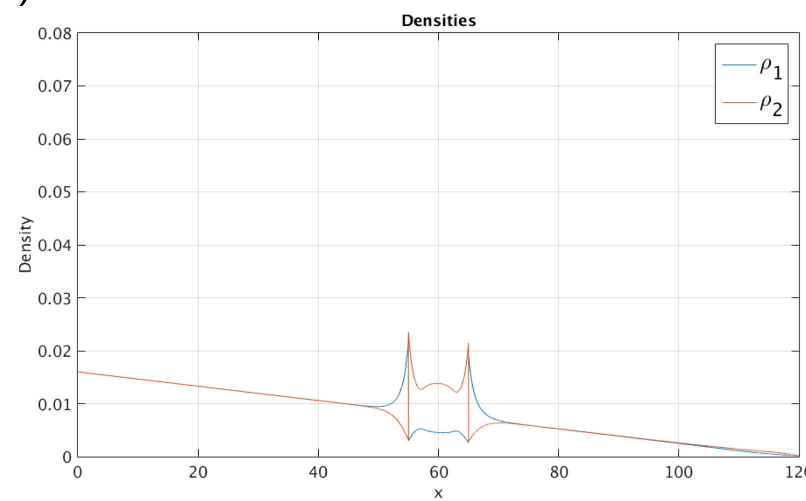
(membrane attracts anions, repels cations)

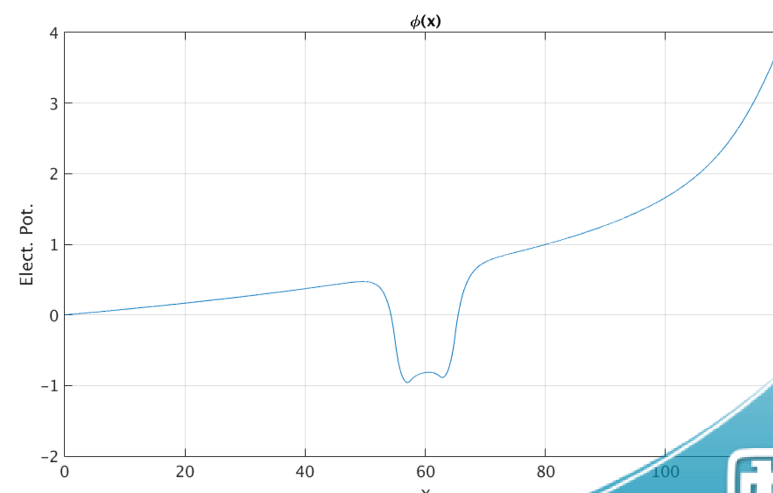
cDFT simulation



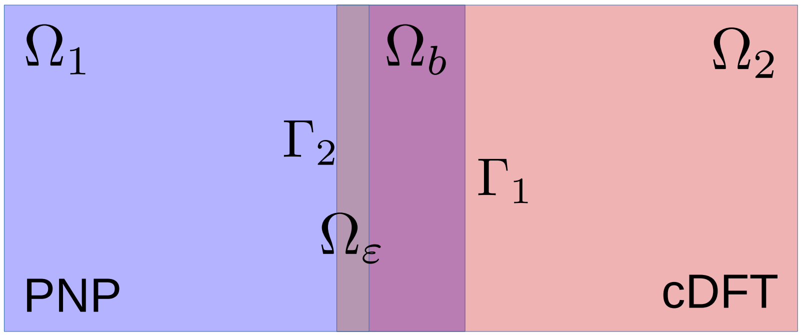


PNP simulation

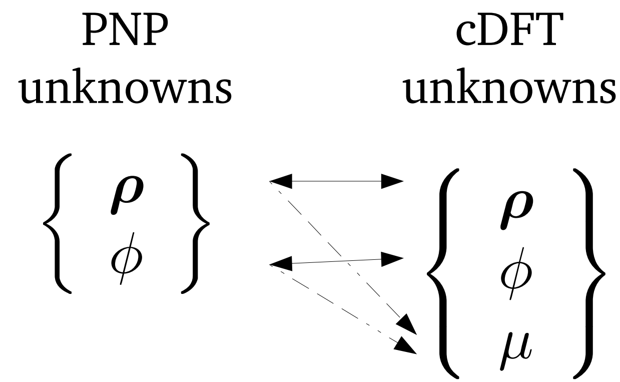




Alternating Schwarz Coupling for PNP-DFT



$$\Omega_b := \Omega_1 \cap \Omega_2$$
$$\Omega_\varepsilon \subset \Omega_1 \cap \Omega_2$$



$$\begin{cases} \mathcal{L}_{\mathrm{PNP}}(\boldsymbol{\rho}_1^{k+1}, \phi_1) = 0 & \text{in } \Omega_1 \\ \boldsymbol{\rho}_1^{k+1} = \boldsymbol{\rho}_2^{k} & \text{on } \Gamma_1 \\ \phi_1^{k+1} = \phi_2^{k} & \text{on } \Gamma_1 \\ \text{other b.c.} & \end{cases}$$

$$\begin{cases} \mathcal{L}_{\mathrm{cDFT}}(\boldsymbol{\rho}_2^{k+1}, \phi_2) = 0 & \text{in } \Omega_2 \\ \boldsymbol{\rho}_2^{k+1} = \boldsymbol{\rho}_1^{k+1} & \boxed{\text{on } \Omega_\varepsilon} \\ \phi_2^{k+1} = \phi_1^{k+1} & \text{on } \Gamma_2 \\ \mu_2^{k+1} = \ln\left(\boldsymbol{\rho}_1^{k+1}\right) + \dfrac{ez}{KT}\phi_1^{k+1} + \left(V + \dfrac{\partial F^{\mathrm{ex}}}{\partial \boldsymbol{\rho}}\right)\left(\boldsymbol{\rho}_1^{k+1}\right) & \text{on } \Gamma_2 \\ \text{other b.c.} & \end{cases}$$

J. Cheung, A. Frishknecht, M. Perego, P. Bochev, in prep, 2016

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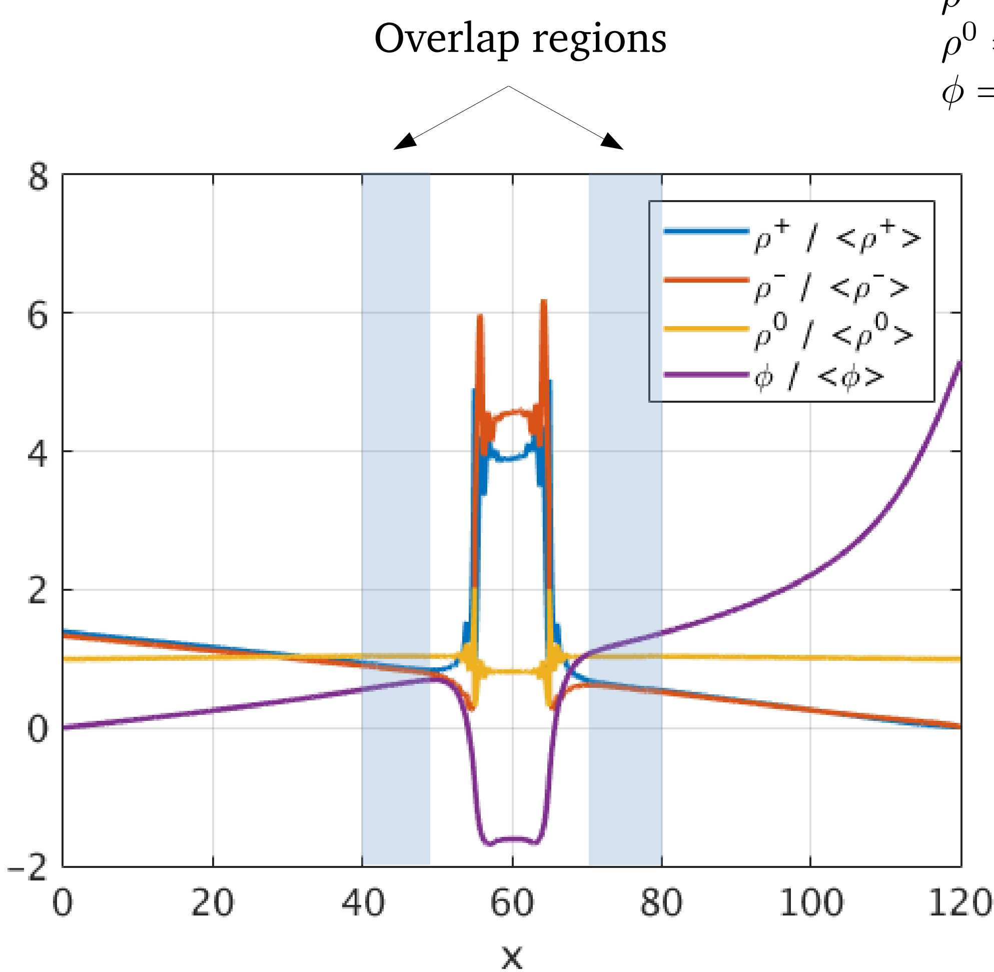
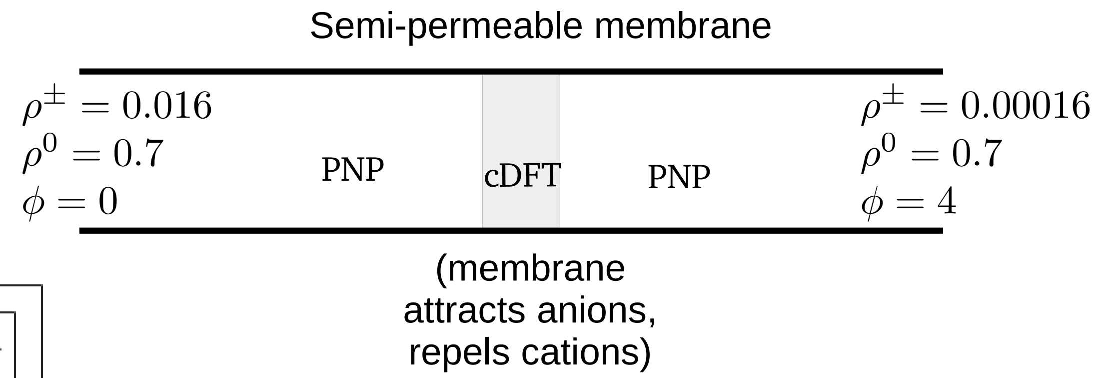
PNP-cDFT Coupling

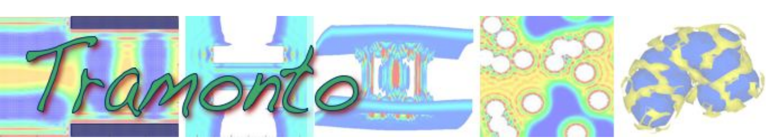




Hybrid solution:

Convergence:

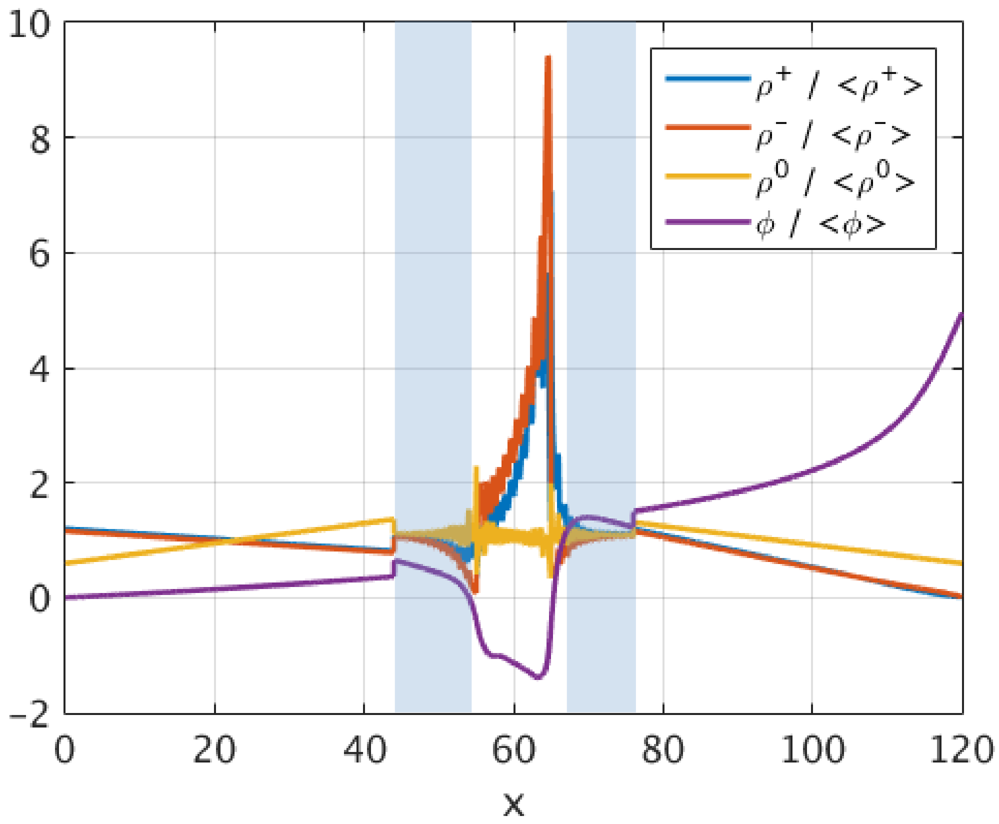
- about 4 iterations converges in “eyeball norm”
- 10 iterations for increment to be less than 1e-4 in L2 norm
- initializing the problem with PNP solved everywhere increases significantly the convergence.



L J Douglas Frink, A Thompson, and A G Salinger. Applying molecular theory to steady-state diffusing systems. J Chem Phys, 2000

PNP-cDFT Coupling

What if we move the overlap region close to the membrane?



- Method is not converging.
- DFT solution is oscillatory next to the membrane and the Dirichlet condition passed to PNP can vary significantly at each iteration

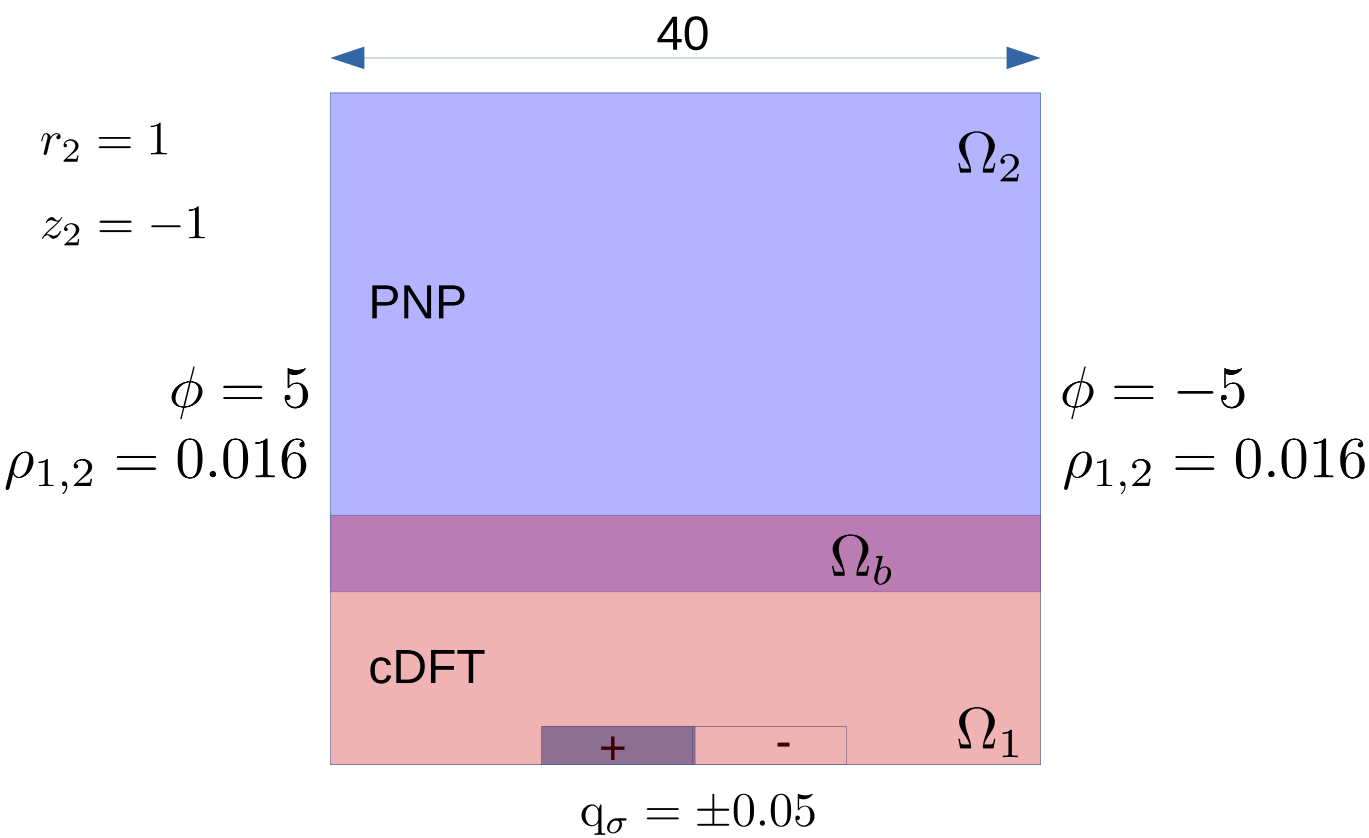
-This is a possible issue with Shwartz coupling. In the following we will present a coupling method that, in principle, should not suffer from this issue.

PNP-cDFT Coupling

2D problem with two monovalent ions:

$r_1 = 2, \qquad r_2 = 1$

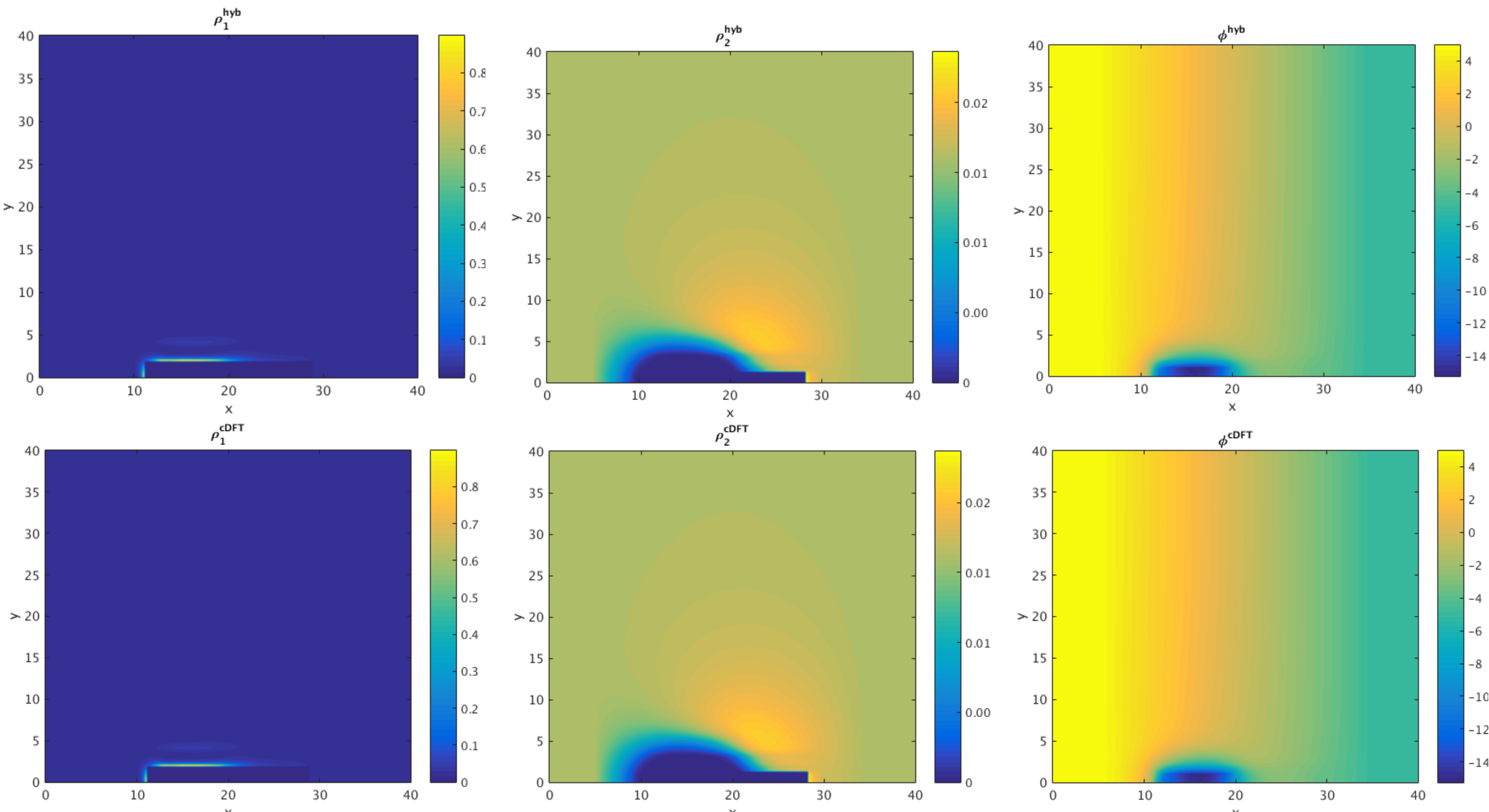
$z_1 = 1, \qquad z_2 = -1$



PNP-cDFT Coupling

Hybrid (PNP-cDFT) solution

Hybrid vs. cDFT: 2x speedup, 0.4x memory usage



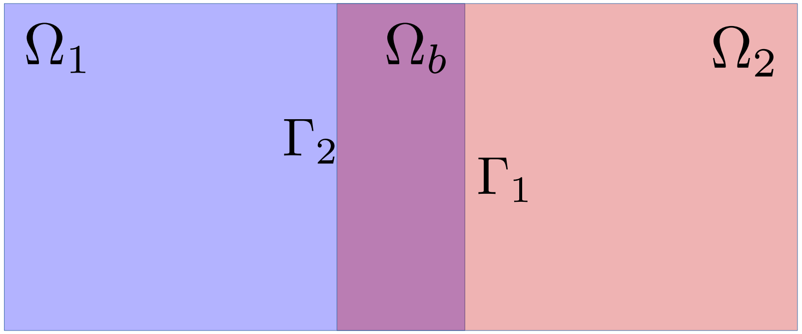
Full cDFT solution

J. Cheung, A. Frishknecht, M. Perego, P. Bochev, in prep, 2016

Optimization-based Coupling

Work by P. Bochev, M. D'Elia, M.Perego, D. Littlewood

Optimization-based Coupling



Research approach: optimization-based coupling:

- Traditional coupling:
  - **Solve the models subject to coupling constraints**
- Optimization coupling reverses the roles:
  - **Minimize coupling error subject to the models**

$$\min_{\boldsymbol{u}_1,\boldsymbol{u}_2,\boldsymbol{\theta}_1,\boldsymbol{\theta}_2} J(\boldsymbol{u}_1,\boldsymbol{u}_2) = \frac{1}{2}\int_{\Omega_b} |\boldsymbol{u}_1 - \boldsymbol{u}_2|^2 \, d\boldsymbol{x} = \frac{1}{2}\|\boldsymbol{u}_1 - \boldsymbol{u}_2\|^2_{0,\Omega_b}$$

s.t.

$$\begin{cases} \mathcal{L}_1(\boldsymbol{u}_1) = 0 & \text{in } \Omega_1 \\ \mathbf{u}_1 = \boldsymbol{\theta}_1 & \text{on } \Gamma_1 \\ \text{other b.c.} & \end{cases} \qquad \begin{cases} \mathcal{L}_2(\boldsymbol{u}_2) = 0 & \text{in } \Omega_1 \\ \boldsymbol{u}_2 = \boldsymbol{\theta}_2 & \text{on } \Gamma_2 \\ \text{other b.c.} & \end{cases}$$

Control variables

Related work: *Lions (2001), Quarteroni (2000), Gunzburger (2000), Du (2001), Hughes (2009), Oden (2011), Karniadakis (2014-Stochastic PDE), Abdulle (2014 – multiscale multiphase flow)*

Optimization-based Coupling

Pros:

- **extremely flexible**
  - Works with non-matching grids, non-coincident interfaces.
  - Coupled models need **not** to share the same discretization, e.g. it can couple finite elements and particle discretizations.
  - Functional to be minimized can be specific of applications, e.g. could be a mismatch of fluxes.
  - Control variables can also be chosen in a fairly arbitrary way (e.g. we can control Neumann conditions)
- Basic idea applicable to diverse modeling scenarios:

  Nonlocal + local electrostatic potential for proteins (CM4), Atomistic-to-continuum coupling.
- Is provably stable & admits rigorous coupling and discretization error analysis.
- At each optimization iteration, models can be solved separately. Good for legacy codes.

Cons:

- It is often more expensive then other coupling strategies
- Requires a fast/robust optimization solver to make the coupling efficient
- Adjoints of the coupled models might be needed to improve convergence

Local to Nonlocal Optimization-based coupling

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

– **M. D'Elia, M. Perego, P. Bochev, D. Littlewood**, A coupling strategy for local and nonlocal diffusion models with mixed volume constraints and boundary conditions, *Computers & Mathematics with Applications*, 2016

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

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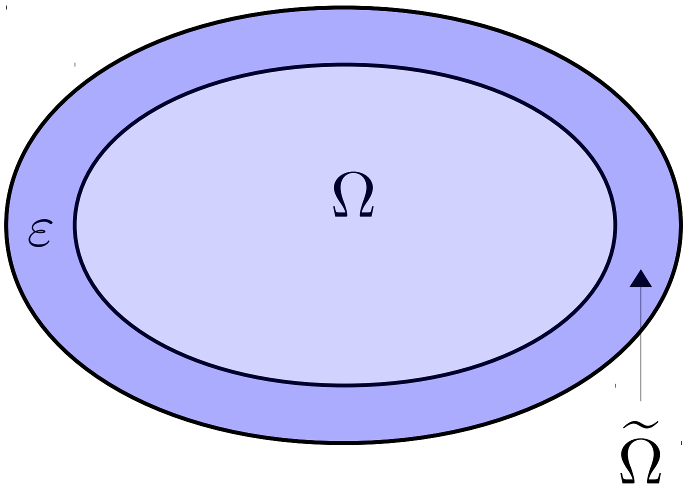
Model Problems

The nonlocal problem



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

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

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

Kernel (depends on material properties)

Kernel: we assume

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

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

Model Problems

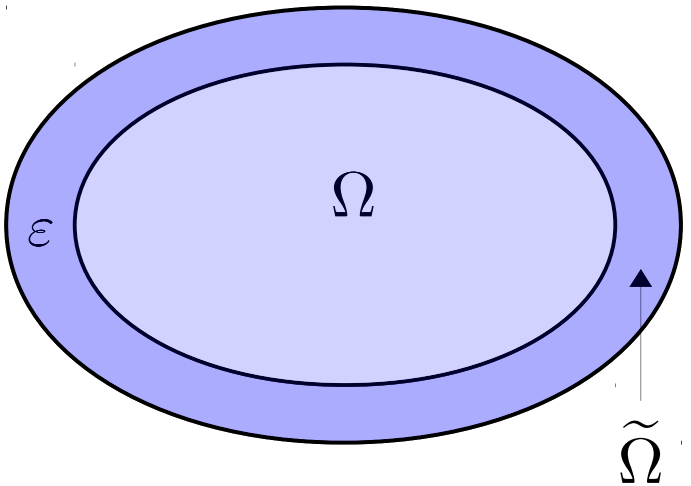
The nonlocal problem

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

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

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

Nonnegative **kernel**
(depends on material properties)

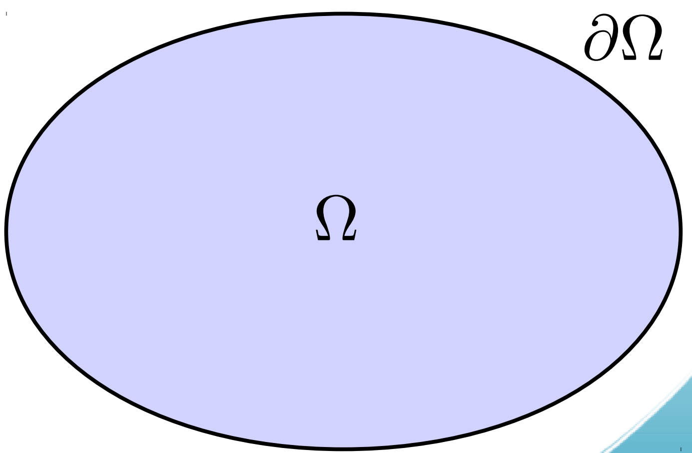


The local problem

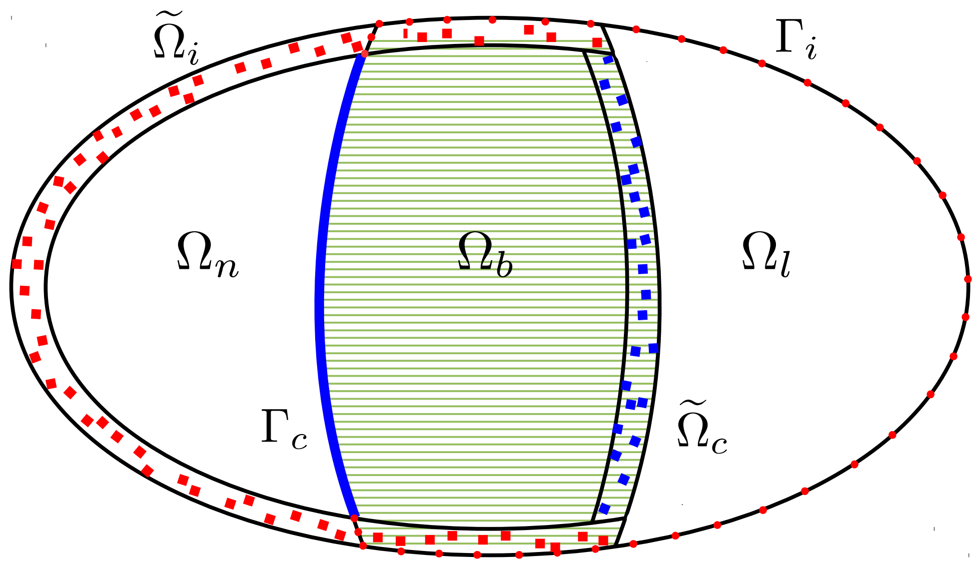
local diffusion model given by the Poisson equation

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

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



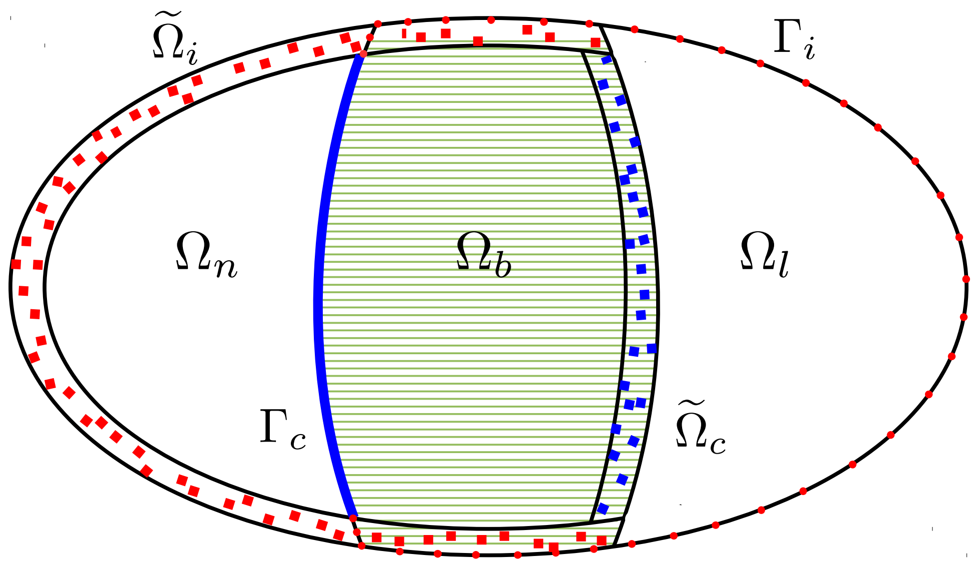
Local to Nonlocal Coupling



State equations:

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

Local to Nonlocal Coupling

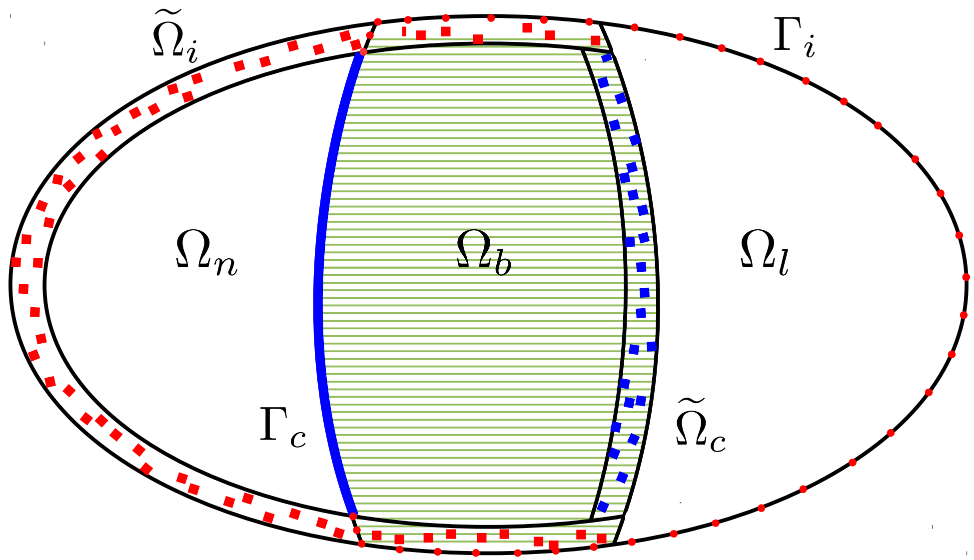


Optimization problem:

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

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

Local to Nonlocal Coupling



Optimization problem:

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

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

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

The Algorithm

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

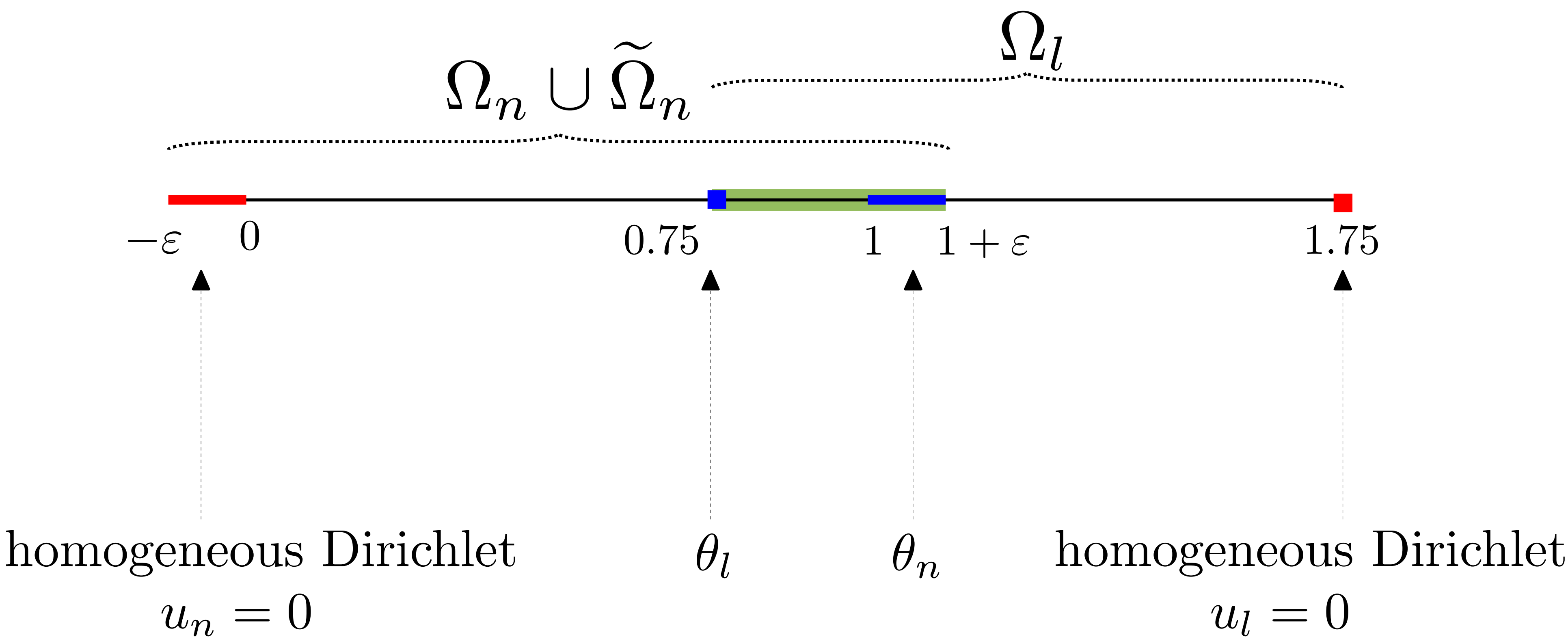
A gradient–based algorithm

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

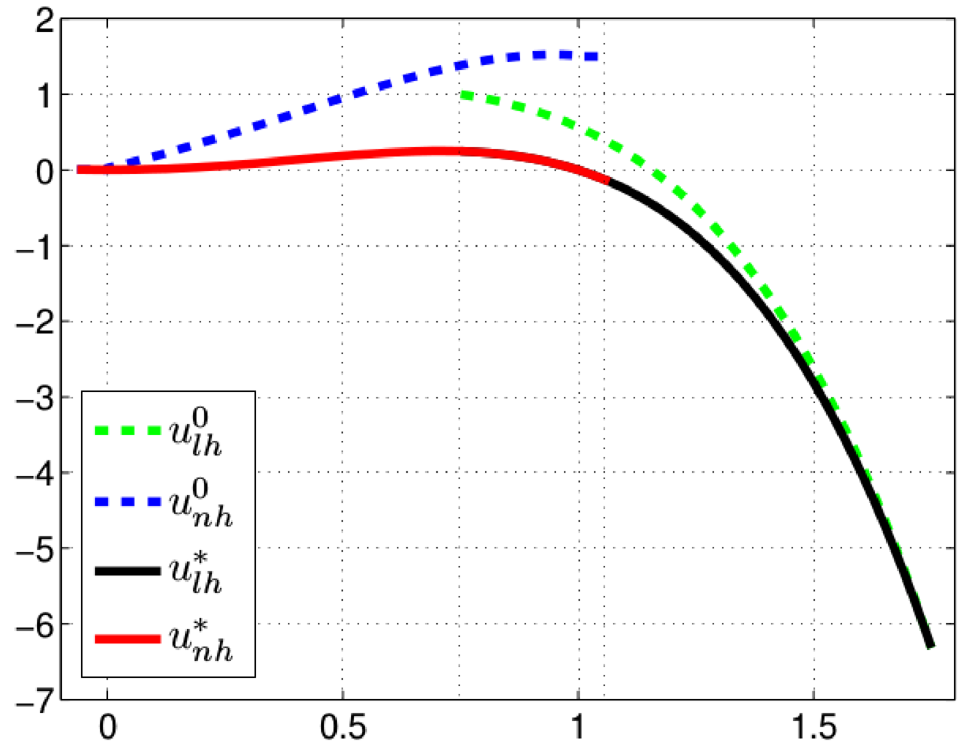
Local to Nonlocal Coupling: Numerical Tests, 1d

Problem Setting (1D)



Numerical Tests

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



Accuracy tests:

- $u_n = u_l = x^2 - x^4$
- $f_n = -2 + 12x^2 + \varepsilon^2$
- $f_l = -2 + 12x^2.$

ε	h	$e(u_n)$	rate	$e(u_l)$	rate	$e(\theta_n)$	rate
	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
0.065	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

Local to Nonlocal Coupling: Numerical Experiment, 3d

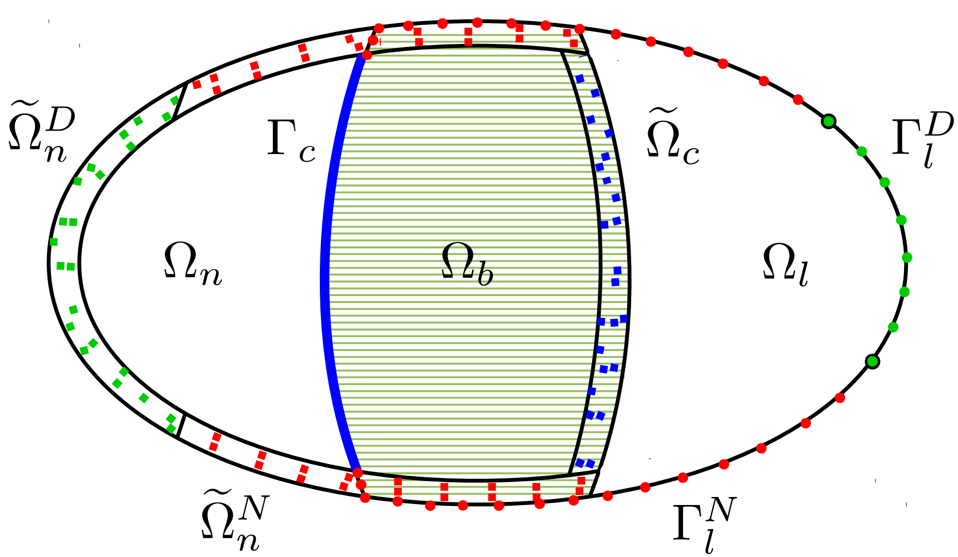
Local to Nonlocal Coupling

Optimization problem:

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

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

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



The Discretization

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

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

strong form + particle method

$$\begin{cases} -\Delta u_l = f_l & \boldsymbol{x} \in \Omega_l \\ u_l = \theta_l & \boldsymbol{x} \in \Gamma_c \\ u_l = 0 & \boldsymbol{x} \in \Gamma_l^D \\ \nabla u_l \cdot \mathbf{n} = 0 & \boldsymbol{x} \in \Gamma_l^N \end{cases}$$

weak form + finite element method

The Discretization

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

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

$$\begin{cases} -\Delta u_l = f_l & \boldsymbol{x} \in \Omega_l \\ u_l = \theta_l & \boldsymbol{x} \in \Gamma_c \\ u_l = 0 & \boldsymbol{x} \in \Gamma_l^D \\ \nabla u_l \cdot \mathbf{n} = 0 & \boldsymbol{x} \in \Gamma_l^N \end{cases}$$

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

$$\mathcal{L}u(\boldsymbol{x}) \approx 2 \sum_{i=1}^{N_{\boldsymbol{x}}} \big(u(\boldsymbol{y}_i) - u(\boldsymbol{x})\big)\, \gamma(\boldsymbol{x}, \boldsymbol{y}_i)\, V_{\boldsymbol{y}_i}$$

The Discretization

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

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

Geometry

Coupling Peridigm and Albany

peridigm.sandia.gov

software.sandia.gov/albany/

trilinos.org/packages/rol

Geometry

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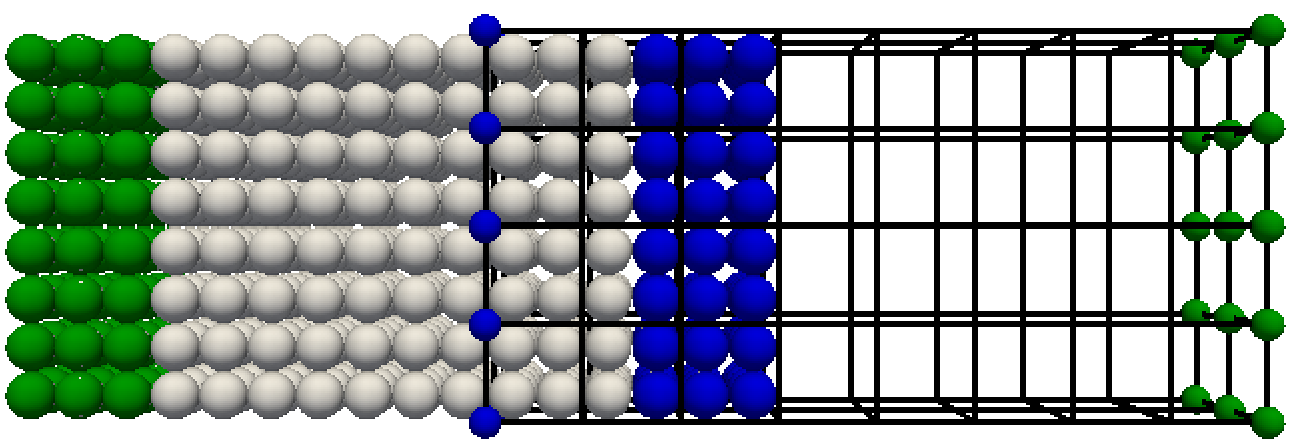


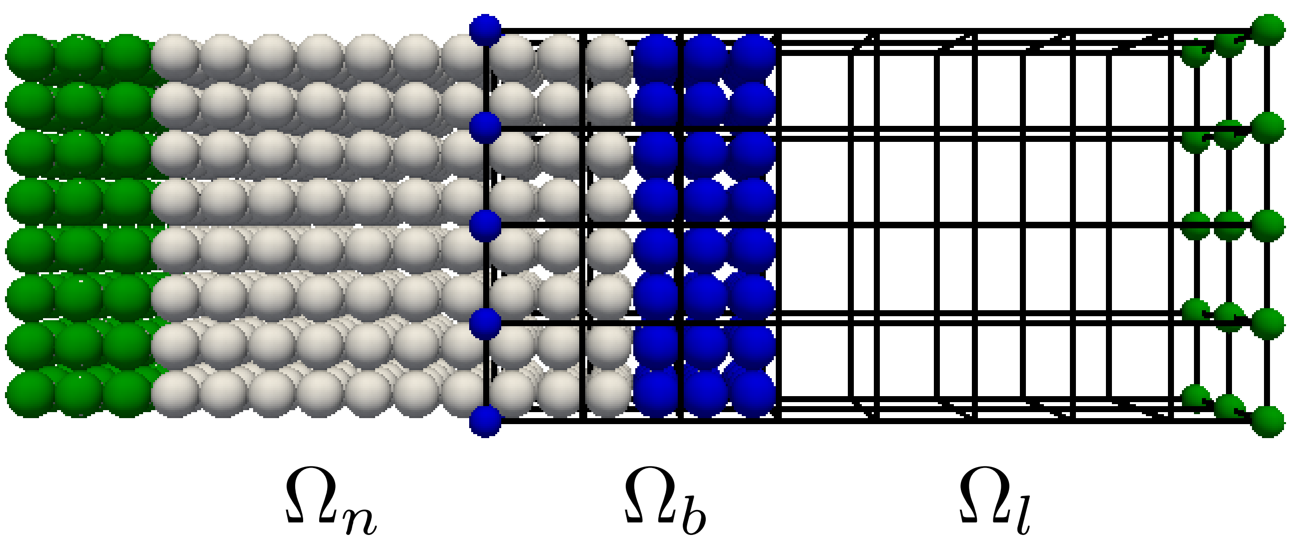
Geometry

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

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

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

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

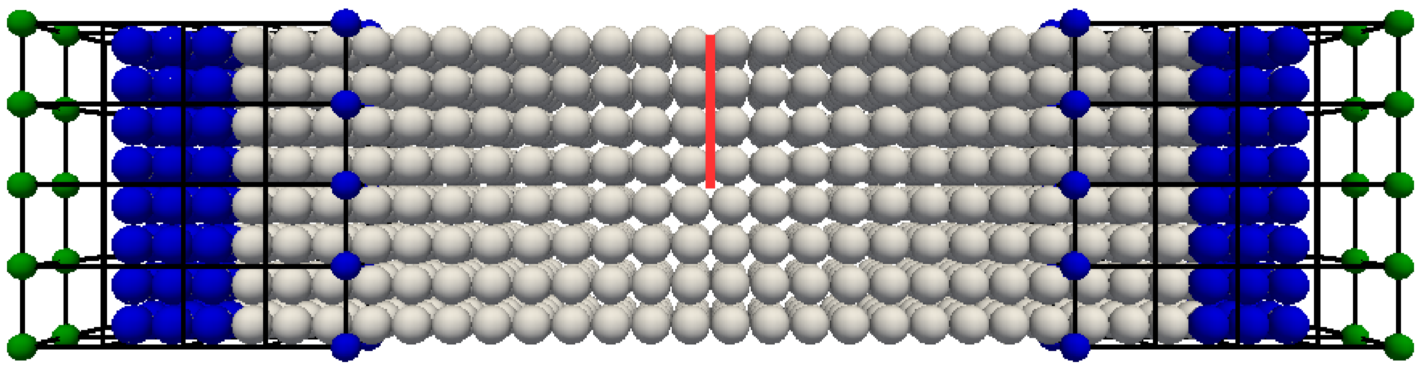


The Patch Test

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

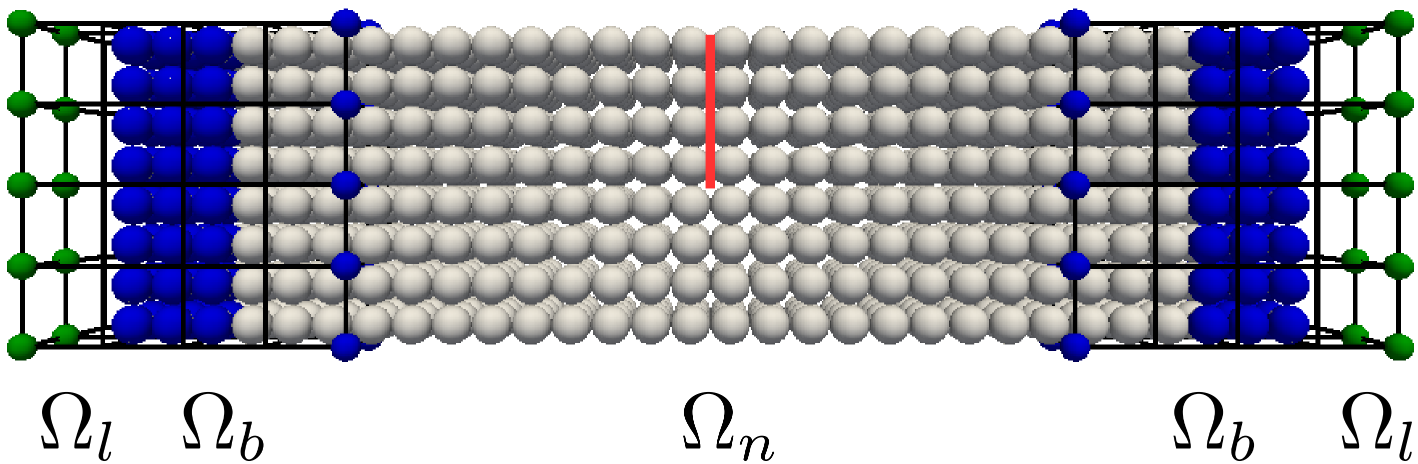
LtN control: initialized at zero in $2 \le x \le 2.5$ and on $x = 1.5$

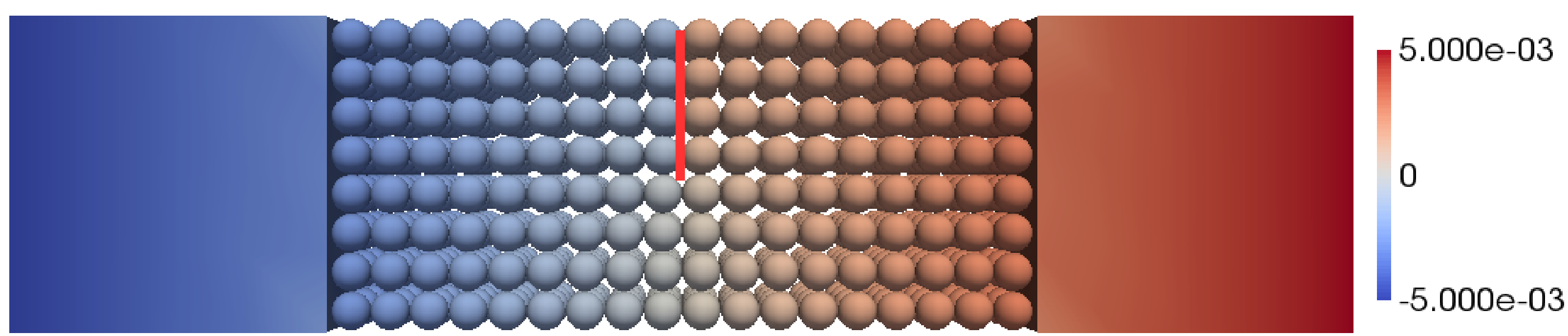
Solution with a Crack



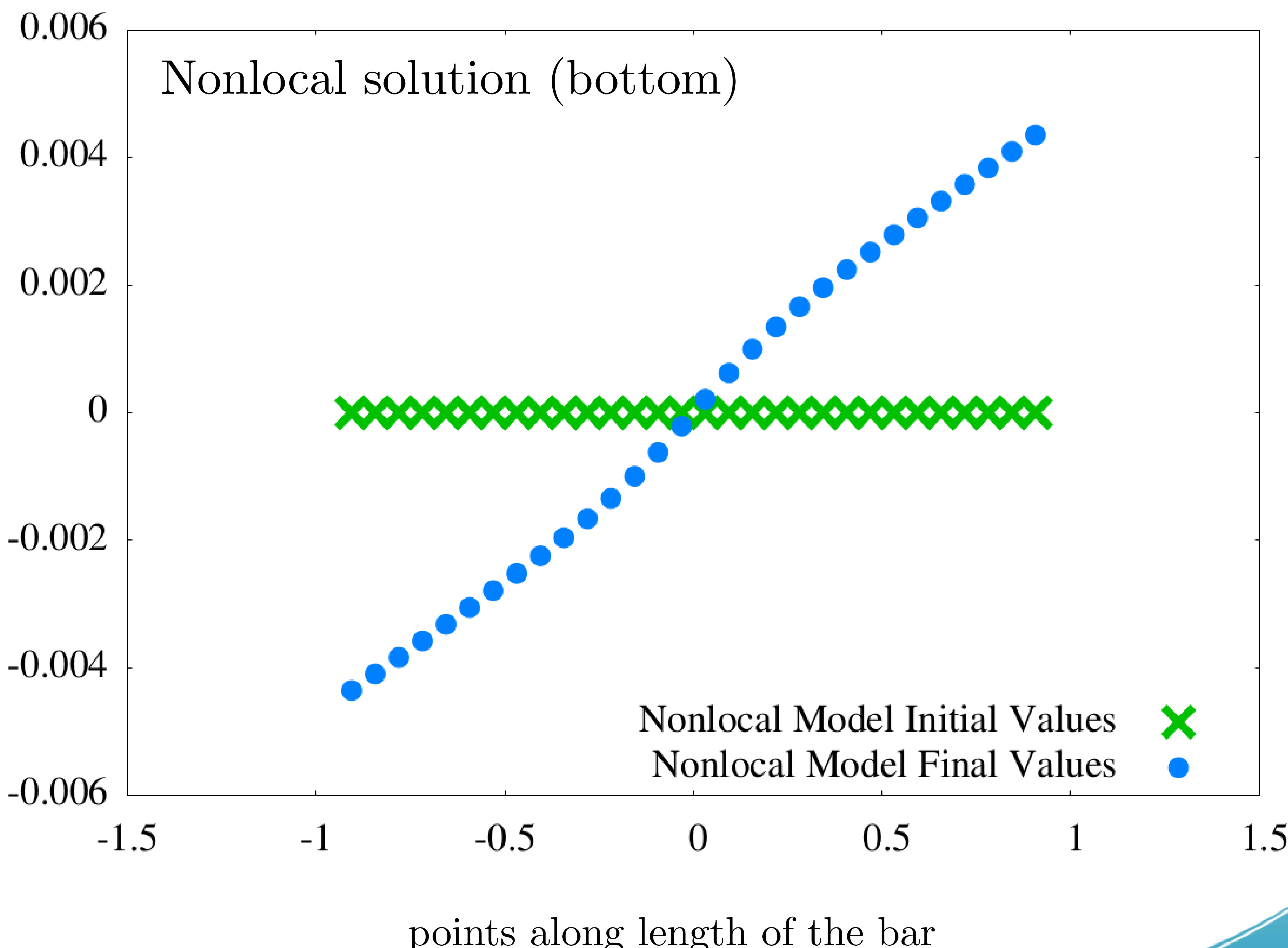
Ω_l Ω_b Ω_n Ω_b Ω_l

Solution with a Crack

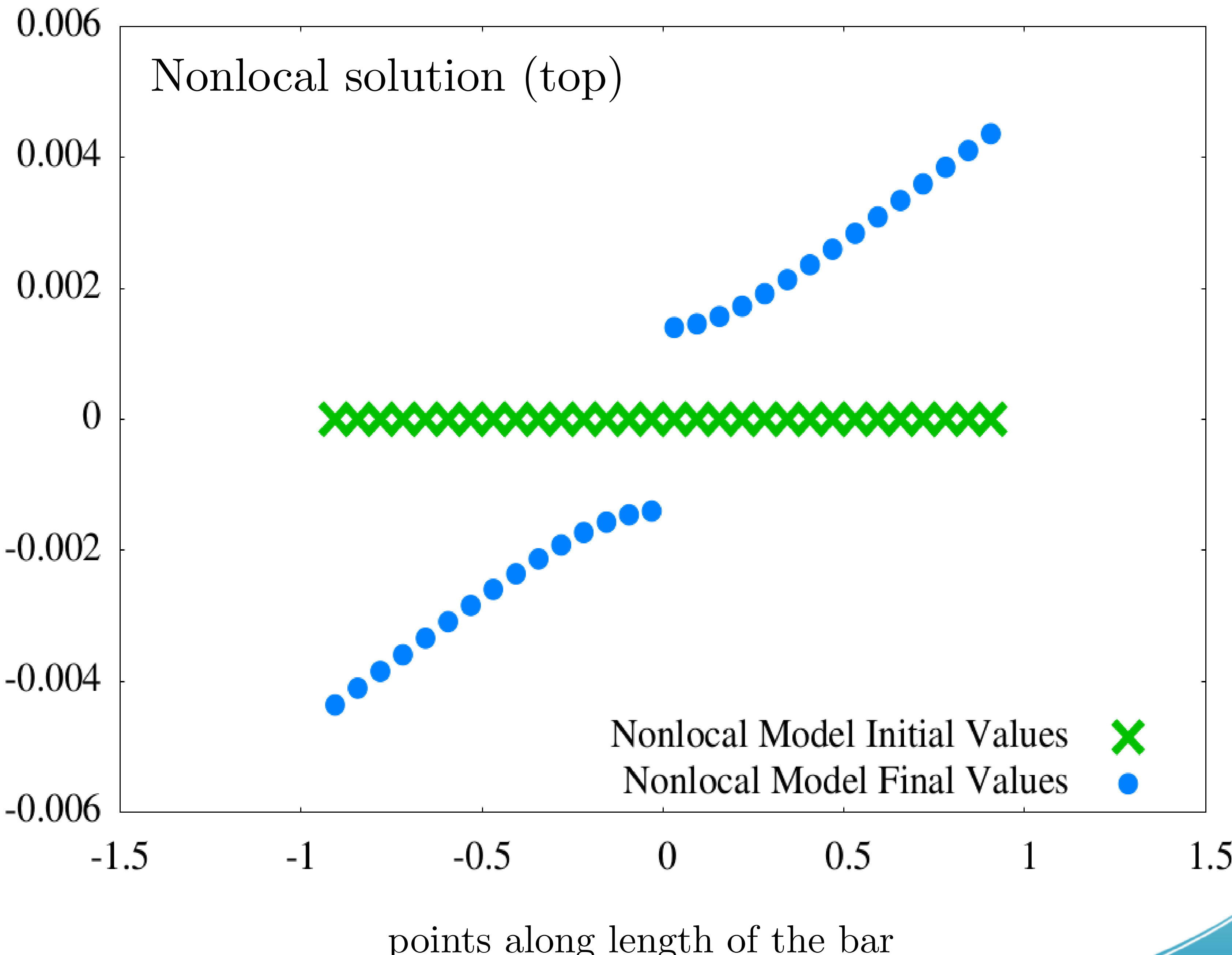




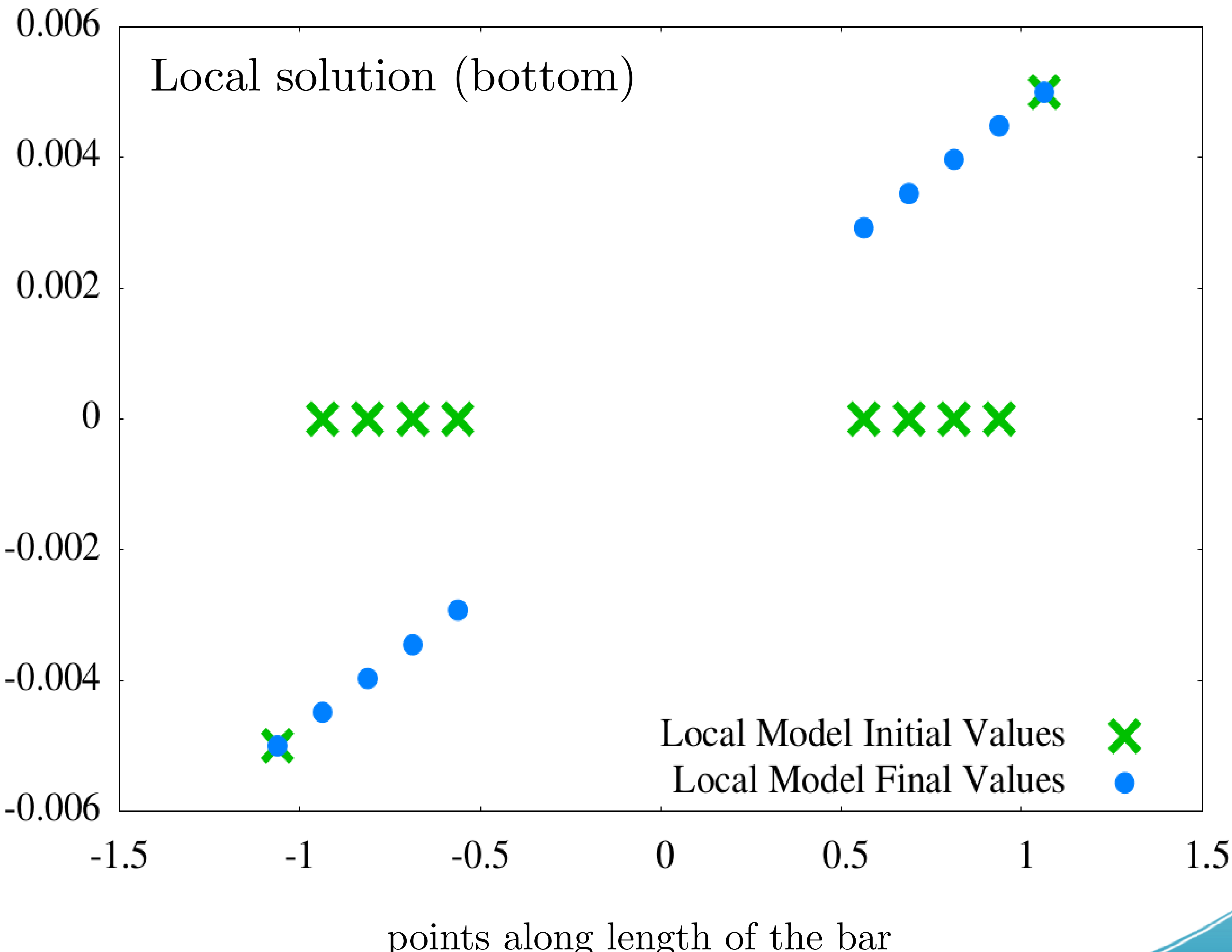
Solution with a Crack



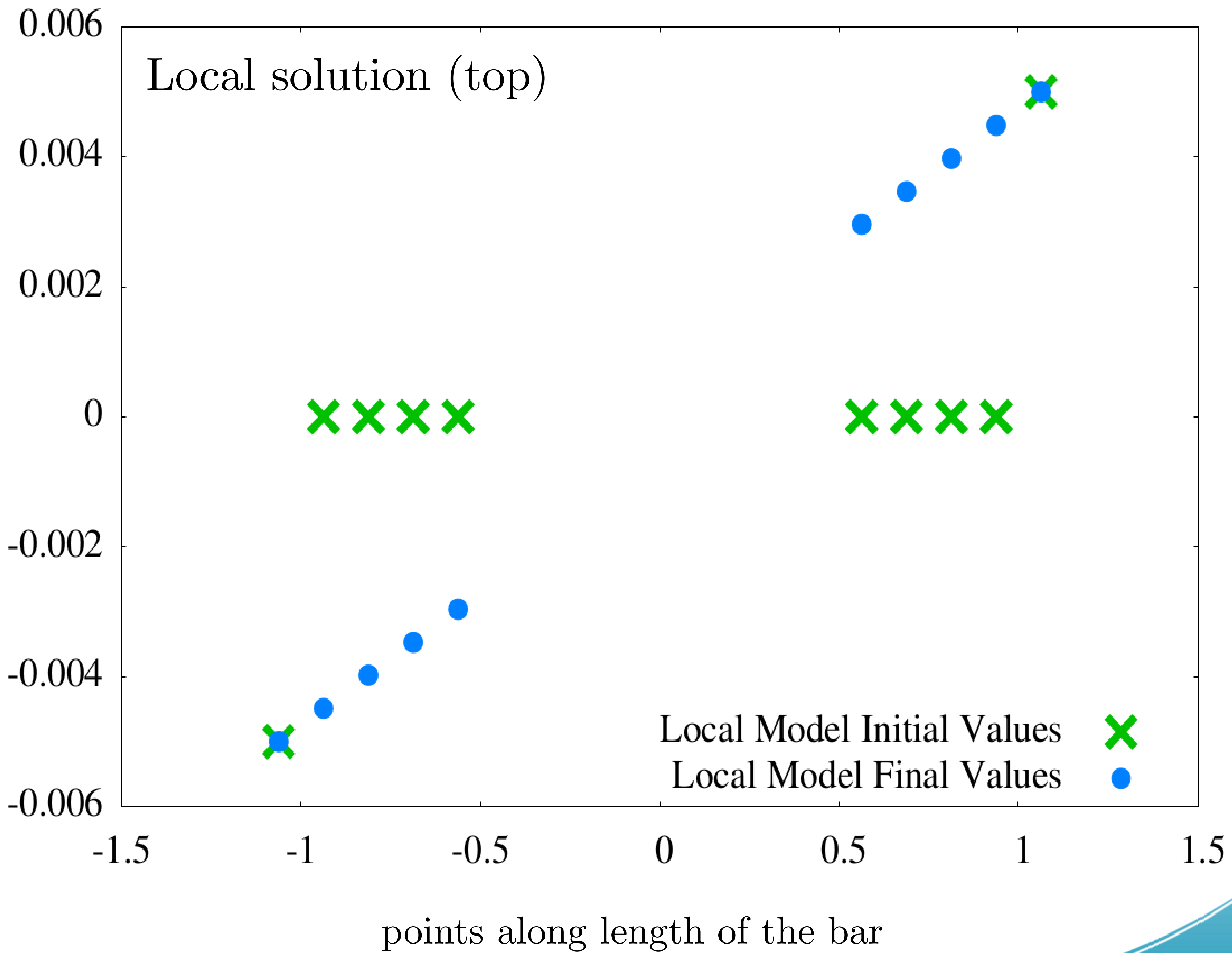
Solution with a Crack



Solution with a Crack



Solution with a Crack



Conclusions

- Presented two nonlocal problems: cDFT and nonlocal Poisson

- Couplings needed to
  1. save computational time,
  2. make feasible (given limited resources) problems too complex to be solved
  3. use legacy codes, e.g. particle methods for nonlocal Poisson and FE for local one.

- Schwarz is in general rather robust but can fail when coupled models behave significantly differently on overlap region.

- Optimization-based coupling is a very general/flexible framework, although it can be expensive.

- Alternative methods not discussed here include the Blending method and the Arlequin method.

Thank you!