Peridynamic Multiscale Finite Element Methods SAND2016-6625C

D. Littlewood[†], T. Costa[†‡], and S. Bond[†]

[†] Center for Computing Research, Sandia National Laboratories,
[‡] Intel Corporation, Hillsboro, Oregon

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Outline

- Motivation
- Peridynamics
- Multiscale Finite Elements
    - Overview
    - Nonlocal Multiscale Finite Elements
    - Mixed-Locality Multiscale Finite Elements
- Analysis: Ambulant Galerkin Framework
- Conclusions & Future Work

Big Picture Goal:

Design scale computational models with quantum accuracy.

Computational Models at Various Scales

- Quantum $\leftarrow$ Density Functional Theory
- Atoms & Molecules $\leftarrow$ Molecular Dynamics
- Molecules to Continuum $\leftarrow$ Peridynamics
- Continuum / Design / Experiment $\leftarrow$ Local PDE

Bridging with Weak Peridynamics

$$DFT \xrightarrow[]{\substack{Machine-Learning\\ IAPs}} MD \xrightarrow[]{\substack{Statistical\\ Coarse-Graining}} PD \xrightarrow{MSFEM} PDE/PD$$

- Let $\Omega \subset \mathbb{R}^d$, $d \in \{1, 2, 3\}$ be a bounded body.
- Any point x interacts directly with any point in $\mathcal{H}_x := \{y \in \Omega \ : \ |x - y| < \delta\}$.
- δ - horizon, $\mathcal{H}_x$ - family of x.

Minimization of Potential Energy → Peridynamic Equation of Motion

$$\rho(x) u_{tt}(x, t) = Lu(x, t) + b(x, t),$$

where L is internal force density,

$$Lu(x, t) = \int_{\mathcal{H}_x} f(u, q, x, t) \, dq.$$

u – displacement field,

ρ – density, reference configuration,

b – external force density,

f – pair-wise bond force density.

[1] S. Silling, Reformulation of elasticity theory for discontinuities and long-range forces, 2001.
[2] S. Silling, M. Epton, O. Weckner, J. Xu, E. Askari, Peridynamic States and Constitutive Modeling, 2007

Linearized Model and Weak Formulation[3,4]

- For small displacements,

$$\rho(x)u_{tt}(x,t) = \int_{\mathcal{H}_x} C(x,q,t)(u(q,t) - u(x,t))\ dq + b(x,t).$$

- $C(x,q,t)$ - tensor-valued micromodulus function, describes linear material.
- Assumes small displacements, but allows material failure.

[3] B. Aksoylu, M. Parks, Variational theory and domain decomposition for nonlocal problems, 2011

[4] X. Chen, M. Gunzburger, Continuous and discontinuous finite element methods for a peridynamics model of mechanics, 2011

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- Multiply to $v \in V$ (to be determined) and integrate to define,

$$\begin{aligned} a(u,v) &= -\int_{\Omega} v(x)\left\{\int_{\mathcal{H}_x} C(x,q)(u(q)-u(x))\,dq\right\}\,dx \\ &= \frac{1}{2}\int_{\Omega}\int_{\mathcal{H}_x} C(x,q)(u(q)-u(x))(v(q)-v(x))\,dq\,dx, \end{aligned}$$

[3] B. Aksoylu, M. Parks, Variational theory and domain decomposition for nonlocal problems, 2011

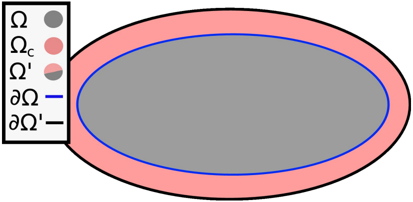
[4] X. Chen, M. Gunzburger, Continuous and discontinuous finite element methods for a peridynamics model of mechanics, 2011

- Define,

$$\|u\|_{\mathcal{E}}^2 = \int_\Omega \int_\Omega C(x,q)(u(q)-u(x))^2 \; dq \; dx,$$

and the energy space

$$\mathcal{E} = \{v : \Omega \to \mathbb{R}^d \;\; : \;\; \|v\|_{\mathcal{E}} < \infty\}.$$



- There is no trace in L^2, problem ill-posed with standard boundary condition.
- The model is nonlocal: consider x with $dist(x, \partial\Omega) < \delta$; x wants more information.

- $\Omega' = \Omega \cup \Omega_c$, where Ω_c is a volume surrounding Ω such that $dist(\partial\Omega, \partial\Omega') \geq \delta$.
- Define $V = \{v \in \mathcal{E} \;\; : \;\; v|_{\Omega_c} = 0\}$.
- Let $\mathcal{A} \in \mathcal{L}(V, V')$ be the operator induced by $a(\cdot,\cdot)$, and write $b(\cdot) = (b, \cdot) \in V'$.
- Weak form, homogeneous Dirichlet peristatic problem:

$$\text{find } u \in V \text{ s.t. } \mathcal{A}u - b = 0 \in V'.$$

[5] M. Gunzburger, R. B. Lehoucq, A nonlocal vector calculus with application to nonlocal boundary value problems, 2010

Multiscale Finite Element Method: Overview

Model problem: FEM for the Dirichlet Poisson Problem

- $\Omega \subset \mathbb{R}^d$, $V = H_0^1(\Omega)$
- $a(u, v) = \int_\Omega \alpha \nabla u \cdot \nabla v$, $f(v) = \int_\Omega Fv$, $F \in L^2(\Omega)$
- $\alpha : \Omega \to \mathbb{R}$ is highly oscillatory, non-degenerate, bounded
- $\mathcal{T}^h$: regular triangularization of Ω, $V^h \subset V$: FEM subspace with basis $\{\phi_i\}_{i=1}^N$

MSFEM Motivation

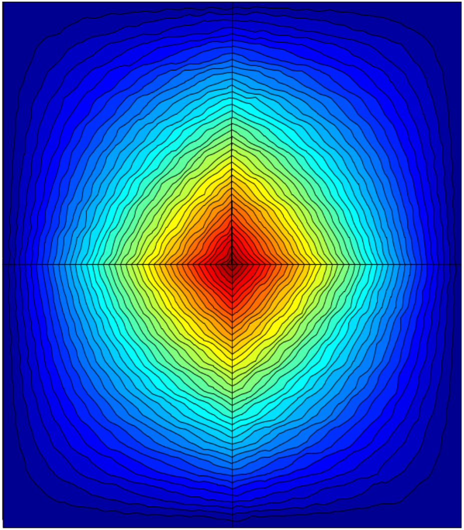
- Resolution required for $\{\phi_i\}_{i=1}^N$ to capture oscillations due to α intractable
- Enhance ϕ_i by a local (element) computation to include α oscillations

MSFEM

- For each $T_i \in \mathcal{T}^h$, define $a_i(u, v) = \int_{T_i} \alpha \nabla u \cdot \nabla v$
- $\mathcal{T}_i^\epsilon$, $V_i^\epsilon \subset H_0^1(T_i)$: triangularization and FEM subspace, respectively
- For each i, and for each ϕ_j with $\text{supp}(\phi_j) \subseteq T_i$

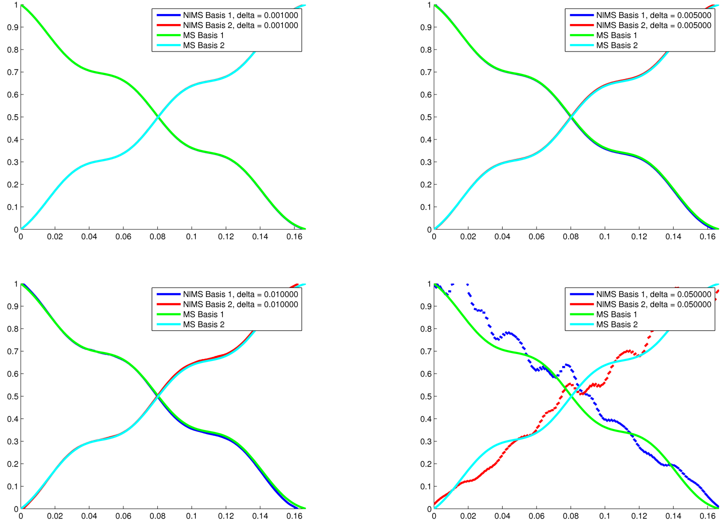
$$\text{find } q_j \in V_i^\epsilon \text{ s.t. } a_i(q_j, v^\epsilon) = -a_i(\phi_j, v^\epsilon), \quad \forall v^\epsilon \in V_i^\epsilon$$

- Define $\phi_j^{MS} = \phi_j + q_j$, and $V_{MS}^h = \text{span}\{\phi_j\}_{j=1}^N$

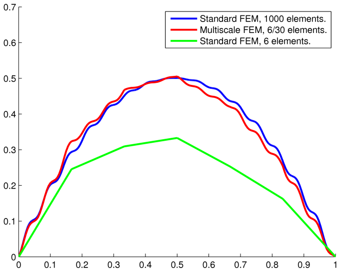


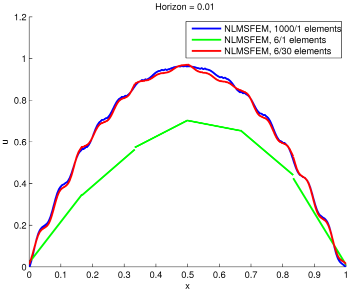
- Multiscale basis function, 2d linear Poisson with periodic heterogeneity and 'hat' functions at both scales
- Image credit: [Y. Efendiev, T. Hou, Multiscale Finite Element Methods, 2009]

- Mesh size: 0.001666, $\alpha(x) = (4 + 3\sin(100x))^{-1}$, $f = 1$.

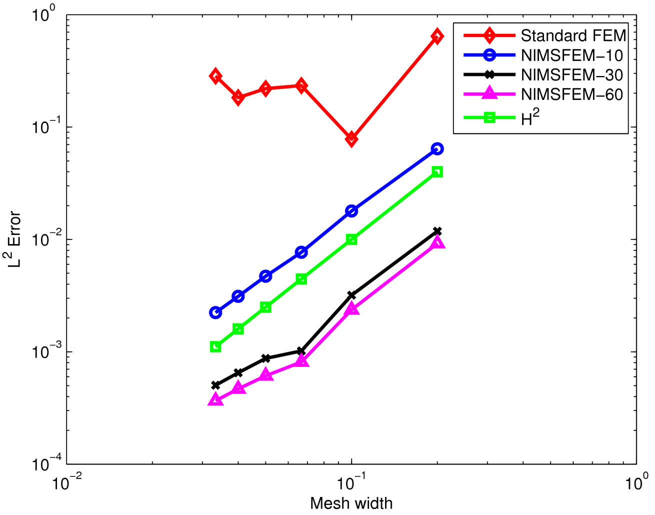


Local and Nonlocal MSFEM

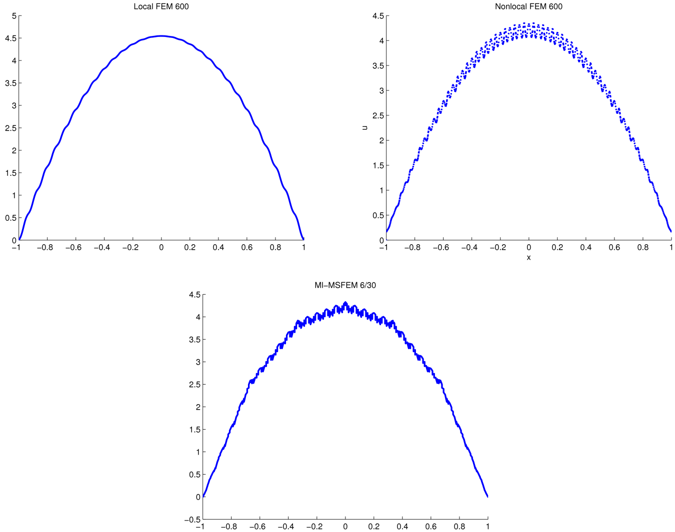




Convergence Tests



Mixed-Locality (An eye ball test)



Model Problem

- Let V be a Hilbert space with inner product $(\cdot,\cdot)$ and norm $\|\cdot\|_V$.
- $\mathcal{B} \in \mathcal{L}(V, V')$: linear, continuous, coercive operator.
- $f \in V'$: continuous linear functional.
- We consider the abstract model problem,

$$\text{find } u \in V \text{ s.t. } \mathcal{B}u - f = 0 \in V'.$$

Ambulant Problem

- $V^H \subset V$, with basis $\{\phi_i\}_{i=1}^{N_H}$ $\leftarrow$ 'approximation space.'
- $I^H : V \to V^H$ $\leftarrow$ projection operator.
- $V^r = Ker(I^H)$ $\leftarrow$ 'residual space.'
- Note: $V = V^H \oplus V^r$.

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- Note: $V = V^H \oplus V^r$.
- 'Reconstruction' $R : V^H \to V$ and 'correction' $Q : V^H \to V^r$ operators defined by,

$$\text{given } \phi \in V^H, \text{ find } Q(\phi) \in V^r \text{ s.t. } \mathcal{B}(\phi + Q(\phi)) - f \in (V^r)^o,$$

and $R(\phi) = \phi + Q(\phi)$.

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  and $R(\phi) = \phi + Q(\phi)$.
- $V^A := \text{span}\{R(\phi_i)\}_{i=1}^{N_H}$ $\leftarrow$ 'ambulant space.'
- Ambulant problem (finite dimensional):

$$\text{find } u^A \in V^A \text{ s.t. } \mathcal{B}u^A - f \in (V^A)^o.$$

Lemma: equivalence of ambulant and weak solutions.

- For any finite dimensional approximation space $V^H \subset V$, the ambulant and weak solutions are equivalent, i.e. $\|u^A - u\|_V = 0$.

- Let $\{V^a\}_a$, $a \in (0, \infty)$ be a family of Hilbert spaces satisfying,
  1. For each a, $V^H \subset V^a \subset V$.
  2. For each $v \in V$ $\exists$ a sequence $\{v^a \in V^a\}_a$ satisfying,
  $$\lim_{a \to 0} \|v - v^a\|_V = 0.$$
- For each a, $V^{r,a} = Ker(I^H|_{V^a})$.
- Define R^a and Q^a by

$$\text{given } \phi \in V^H, \text{find } Q^a(\phi) \in V^{r,a} \text{ s.t. } \mathcal{B}(\phi + Q^a(\phi)) - f \in (V^{r,a})^o,$$

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Ambulant Galerkin Method

Define $V^{A_a} = \text{span}\{R^a(\phi_i)\}_{i=1}^{N_H}$, then

find $u^{ag} \in V^{A_a}$ s.t

$$\mathcal{B}u^{ag} - f \in (V^{A_a})^o.$$

Ambulant Petrov-Galerkin Method

Define $V^{A_a} = \text{span}\{R^a(\phi_i)\}_{i=1}^{N_H}$, then

find $u^{apg} \in V^{A_a}$ s.t

$$\mathcal{B}u^{apg} - f \in (V^H)^o.$$

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Define $V^{A_a} = \text{span}\{R^a(\phi_i)\}_{i=1}^{N_H}$, then

$$\text{find } u^{ag} \in V^{A_a} \text{ s.t}$$
$$\mathcal{B}u^{ag} - f \in (V^{A_a})^o.$$

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Define $V^{A_a} = \text{span}\{R^a(\phi_i)\}_{i=1}^{N_H}$, then

$$\text{find } u^{apg} \in V^{A_a} \text{ s.t}$$
$$\mathcal{B}u^{apg} - f \in (V^H)^o.$$

Theorem 1: AG Convergence

$$\lim_{a\to 0} \|u - u^{ag}\|_V = 0.$$

Theorem 2: APG Convergence

$$\lim_{a\to 0} \|u - u^{apg}\|_V = 0.$$

Why 'ambulant': how does AFEM translate the problem on V^H?

- Let $\{\psi_i\}_{i=1}^{N_a}$ be a basis for $V^{r,a}$ and let $\{w_{ij}\}_{ij}$, $1 \leq i \leq N_H$, $1 \leq j \leq N_a$ be defined by,

$$R^a(\phi_i) = \sum_{j=1}^{N_a} w_{ij}\psi_j.$$

- Define,

$$\begin{aligned}
\mathbf{B}^H \in \mathbb{R}^{N_H \times N_H} &: \mathbf{B}^H_{ij} = \mathcal{B}\phi_i(\phi_j),\\
\mathbf{B}^{pg} \in \mathbb{R}^{N_H \times N_H} &: \mathbf{B}^{pg}_{ij} = \mathcal{B}R^a(\phi_i)(\phi_j),\\
\mathbf{B}^{g} \in \mathbb{R}^{N_H \times N_H} &: \mathbf{B}^{g}_{ij} = \mathcal{B}R^a(\phi_i)(R^a(\phi_j)),\\
\mathbf{B}^{r,a} \in \mathbb{R}^{N_a \times N_a} &: \mathbf{B}^{r,a}_{ij} = \mathcal{B}\psi_i(\psi_j),\\
\mathbf{B}^{L} \in \mathbb{R}^{N_a \times N_H} &: \mathbf{B}^{L}_{ij} = \mathcal{B}\psi_i(\phi_j),\\
\mathbf{B}^{R} \in \mathbb{R}^{N_H \times N_a} &: \mathbf{B}^{R}_{ij} = \mathcal{B}\phi_i(\psi_j),\\
\mathbf{W} \in \mathbb{R}^{N_H \times N_a} &: \mathbf{W}_{ij} = w_{ij}.
\end{aligned}$$

Then,

$$\mathbf{B}^g = \mathbf{B}^H + \mathbf{B}^R\mathbf{W}^T + \mathbf{W}\mathbf{B}^L + \mathbf{W}\mathbf{B}^{r,a}\mathbf{W}^T,$$

and

$$\mathbf{B}^{pg} = \mathbf{B}^H + \mathbf{W}\mathbf{B}^L.$$

AFEM as ROM: how does AFEM reduce the problem on V^a?

- Define a basis for V^a, $\{\theta_i\}_{i=1}^{N_H+N_a}$,

$$\theta_i = \begin{cases} \phi_i & 1 \leq i \leq N_H, \\ \psi_{i-N_H} & N_H + 1 \leq N_H + N_a \end{cases} .$$

- Then define,

$$\mathbb{B} \in \mathbb{R}^{(N_H+N_a)\times(N_H+N_a)} : \mathbb{B}_{ij} = \mathcal{B}\theta_i(\theta_j),$$
$$\mathbb{W} \in \mathbb{R}^{N_H\times(N_H+N_a)} : \mathbb{W}_{ij} = \begin{cases} \delta_{ij} & j \leq N_H \\ w_{i(j-N_H)} & j > N_H \end{cases} ,$$

or in blocks,

$$\mathbb{B} = \begin{pmatrix} \mathbf{B}^H & \mathbf{B}^R \\ \mathbf{B}^L & \mathbf{B}^{r,a} \end{pmatrix}, \quad \mathbb{W} = \begin{pmatrix} \mathbf{I}_{N_H} \\ \mathbf{W} \end{pmatrix}.$$

- Then,

$$\mathbf{B}^g = \mathbb{W}\mathbb{B}\mathbb{W}^T,$$

and

$$\mathbf{B}^{pg} = \mathbb{W}\mathbb{B}\begin{bmatrix} \mathbf{I}_{N_H} & 0 \end{bmatrix}.$$

- V: functional space whose elements are defined on $\mathbb{R}^d$.
- V^H is now a low DOFs finite element space.

Obtaining MSFEM from AFEM

1. Define the mesh in V^a as a regular mesh refinement of the mesh in V^H.
2. Restrict computation of $R^a(\phi_i)$ to the support of ϕ_i.
3. Disregard f in computation of $R^a(\phi_i)$.

- Error induced by 2 and 3 (Controlled by H).

Theorem 3: Source Removal →Orthogonality Preserving Translation

The map $\phi \to R^a(\phi) = \phi + Q^a(\phi)$ where $Q^a(\phi)$ is defined by,

$$\text{find } Q^a(\phi) \in V^{r,a} \text{ s.t. } \mathcal{B}(\phi + Q^a(\phi)) \in (V^{r,a})^o,$$

is orthogonality preserving. In particular, if $\{\phi_i\}_{i=1}^{N_H}$ is an orthogonal basis for V^H, then $\{R^a(\phi_i)\}_{i=1}^{N_H}$ is an orthogonal basis for V^{A_a}.

Conclusions & Future Work

Conclusions

- Demonstrated MSFEM performance for linear Peridynamic model in 1d
- Demonstrated MSFEM performance for mixed nonlocal-local coupling between scales
- Introduced AGM as a strategy for mathematical analysis of MSFEM for local and nonlocal models

Future Work

- 2d/3d
- Nonlinear constitutive models
- Analysis of mixed-locality method with AGM