Material-adapted Refinable Basis Functions for Elasticity Simulation

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Motivation

Inhomogeneity everywhere...

Simulating inhomogeneous material objects can be very challenging

- Large scales
- Poor condition

Homogenization!

Organs, compounds, metamaterials...
Homogenization (Coarse-graining)

• Fitting locally-homogeneous model

**Numerical Coarsening of Inhomogeneous Elastic Materials**
Lily Khareyevych, Patrick Mullen, Houman Owhadi, Mathieu Desbrun

Abstract
We propose an approach for efficiently simulating elastic objects made of non-homogeneous, non-isotropic materials. Based on recent developments in homogenization theory, a methodology is introduced to approximate a heterogeneous object made of arbitrary fine.

**Data-Driven Finite Elements for Geometry and Material Design**
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**Mechanical Characterization of Structured Sheet Materials**
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• Idea
  ➢ “Average” the inhomogeneous potential functional from fine to coarse

• Limitations
  ➢ Hard to encode general anisotropy for nonlinear problems
  ➢ Limited ability to capture complex anisotropic behavior
Homogenization (Coarse-graining)

- **Idea**
  - Optimize coarse-to-fine “prediction” by adapting the bases to the inhomogeneity

- **Limitations**
  - Limited expressivity for elasticity
  - Not flexible enough to handle arbitrary coarse scale
  - Cost much to compute
How basis functions play a role

PDE
\[ \mathcal{L} : H \rightarrow H^* \]
linear
self-adjoint
positive-definite

Introduce test function
\[ \forall v \in H \]

Weak form
\[ L(u, v) := \int L(u) \cdot v \]

A set of basis fcts for testing
\[ \{ \phi_i \}_i \]

Lax-Milgram theorem ensures the unique solution for any RHS

Linear Eqns
\[ A_{ij} u_j = b_i \]
\[ A_{ij} = L(\phi_i, \phi_j) \]
\[ b_i = G(\phi_i) \]
Choosing basis functions

- Global basis functions
  - Eigenfunctions (modal basis)
    - Pros
      - Complete scale separation
      - Spectral convergence
      - Effective reduction
    - Cons
      - No associated spatial DoFs
      - Expensive to compute

- Local basis functions
  - Low-order polynomial basis
    - Pros
      - Simple, efficient and generalizable
      - Friendly to boundary conditions
    - Cons
      - Poor convergence for even homogeneous problem
      - Bad conditioning

Can we bridge two extremes?
Sparse optimization approach

• [Brandt and Hildebrandt 2017]

\[
\begin{align*}
\mathbf{u}_i & := \arg \min_{\mathbf{u}} \quad \mathbf{u}^T \mathbf{H} \mathbf{u} + \mu \| \mathbf{u} \|_1 \\
\text{subject to} \quad & \mathbf{u}^T \mathbf{M} \mathbf{u} = 1 \quad \text{and} \quad \forall j < i : \mathbf{u}^T \mathbf{M} \mathbf{u}_j = 0
\end{align*}
\]

• Complicated nonlinear optimization
• Not intuitive to control the locality
**MultiResolution Analysis (MRA)**

- Hierarchical orthogonal decomposition
  \[ \mathcal{V}^{k+1} = \mathcal{V}^k \oplus \mathcal{W}^k \]
  \[ \mathcal{V}^q = \mathcal{V}^1 \oplus \mathcal{W}^1 \oplus \ldots \oplus \mathcal{W}^{q-1} \]

- Multiresolutional basis functions
  \[ \mathcal{V}^{k+1} = \text{span}(\varphi_{i}^{k+1}) \oplus \text{span}(\varphi_{i}^{k}) \oplus \text{span}(\psi_{j}^{k}) \]
  \[ \forall i, j, \int \varphi_{i}^{k} \psi_{j}^{k} = 0 \]

Wavelets

Scaling functions
MultiResolution Analysis (MRA)

• Multiresolutional upsampling

\[ u^q(x) = \sum_{i} v_i^1 \varphi_i^1(x) + \sum_{k=1}^{q-1} \sum_{j} w_j^k \psi_j^k(x) \]

• Stiffness matrix structure

\[
\begin{bmatrix}
A^1 := L(\varphi^1, \varphi^1) & L(\varphi^1, \psi^1) & \cdots & L(\varphi^1, \psi^{q-1}) \\
L(\psi^1, \varphi^1) & B^1 := L(\psi^1, \psi^1) & \cdots & L(\psi^1, \psi^{q-1}) \\
\vdots & \vdots & \ddots & \vdots \\
L(\psi^{q-1}, \varphi^1) & L(\psi^{q-1}, \psi^1) & \cdots & B^{q-1} := L(\psi^{q-1}, \psi^{q-1})
\end{bmatrix}
\]
Orthogonality

Why $L_2$-orthogonality?

**Operator-orthogonal decomposition**

\[
\begin{align*}
\mathcal{V}^{k+1} &= \mathcal{V}^k \oplus L \mathcal{W}^k \\
\text{span}(\varphi_i^{k+1}) &\quad \text{span}(\varphi_i^k) \quad \text{span}(\psi_j^k)
\end{align*}
\]

\[
\forall i, j, \int \varphi_i^k L \psi_j^k = 0
\]

**Block diagonal stiffness matrix**

\[
L = \begin{pmatrix}
A^1 & 0 & \cdots & 0 \\
0 & B^1 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & B^{q-1}
\end{pmatrix}
\]

*Clustered scale separation*
Spatial locality

Besides, we want the basis functions to be locally supported

- to be able to capture local deformation
- to handle boundary conditions properly
- to sparsify the system matrix for computational efficiency
Construction for elasticity
Mesh hierarchy

- Loose requirement on mesh hierarchy...
  - Simplicial/polyhedral
  - Nested/non-nested
  - Subdivision/aggregation
Refinable basis functions

• ...as long as the associated basis functions are **refinable**

\[ \forall k \in \{1, \ldots, q-1\}, \quad \varphi_i^k = \sum_{j=1}^{n_{k+1}} C_{ij}^k \varphi_j^{k+1}, \quad C_i^k \]

- Refinement kernel \( W \)

\[ C^k W^k, T = 0 \]

**\( L_2 \) orthogonal by construction**
Matrix-valued extension

• Matrix-valued basis functions [Chen 2018]

For any level $k$

$$\phi_i^k : \Omega \rightarrow \mathbb{R}^{d \times d}$$

Finest level

$$\phi_i^q(x) = \begin{bmatrix} \bar{\phi}_i(x) & 0 & 0 \\ 0 & \bar{\phi}_i(x) & 0 \\ 0 & 0 & \bar{\phi}_i(x) \end{bmatrix}$$

Idea: provide sufficient DOFs to encode local anisotropy.

• Matrix dimensions

$$C_{ij}^k, W_{ij}^k \in \mathbb{R}^{3 \times 3}$$

$$C^k \in \mathbb{R}^{3n_k \times 3n_{k+1}}$$

$$W^k \in \mathbb{R}^{(3n_{k+1} - 3n_k) \times 3n_{k+1}}$$
Material-adapted refinement

Material **blind** MR bases

$$\varphi_i^k = \sum_{j=1}^{n_{k+1}} C_{ij}^k \varphi_j^{k+1}$$

$$\psi_i^k = \sum_{j=1}^{n_{k+1}} W_{ij}^k \varphi_j^{k+1}$$

**Bootstrapping**

$$\varphi_i^q \equiv \varphi_i^q$$

Material **adapted** MR bases

$$\varphi_i^k = \sum_{j=1}^{n_{k+1}} C_{ij}^k \varphi_j^{k+1}$$

$$\psi_i^k = \sum_{j=1}^{n_{k+1}} W_{ij}^k \varphi_j^{k+1}$$

To be solved...
L-orthogonality

Enforce orthogonality w.r.t. metric $\mathcal{L}$

$$\int_{\Omega} \phi_i^k \mathcal{L} \psi_j^k, T = 0 \quad \forall i, j,$$

$$C^k A^{k+1} W^k, T = 0$$
Spatial locality

Enforce collocation with non-adapted local basis functions

\[ \int_{\Omega} \varphi_{i}^{k} \varphi_{j}^{k} = \delta_{ij} \quad \forall i, j, \]

\[ C_{k}^{k}, T = I \]
Variational formulation

Equivalent variational formulation

\[ \varphi_i = \arg \min_{\phi} \int_\Omega \phi \mathcal{L} \phi \quad \text{s.t.} \quad \int_\Omega \phi \varphi_j = \delta_{ij} \quad \forall j. \]

[Refer to our paper for a proof]

Discrete form

\[ C^k = \arg \min_M \text{Tr}[MA^{k+1}M^T] \quad \text{s.t.} \quad MC^{k,T} = I_{3n_k \times 3n_k}. \]

[A simple quadratic problem]

Close-formed solution

\[ C^k = C^{k, \dagger} \left[ I_{3n_{k+1} \times 3n_{k+1}} - A^{k+1} W^{k,T} \left( B^k \right)^{-1} W^k \right], \]

[Recursively applied for multilevel decomposition]
Hierarchical adapted basis fcts
Hierarchical adapted basis fcts
Hierarchical adapted basis fcts & wavelets
Spectrum and conditioning

Bilinear

Dirac

Eigen ranges

condition number

level

coarser

finer
Basis truncation

• The coarser the level is, the larger support region basis functions will have, which slows down
  • Matrix factorization
  • Matrix multiplication

• Fast decay property allows for truncation of the basis functions
  • See our paper for details

• Besides, geometrical invariance should be preserved

\[
\forall j, \sum_i C^k_{ij} = I_{3\times3},
\]

translation

\[
\forall j, \sum_i C^k_{ij} [\bar{x}_i^{k-1}]_x = [\bar{x}_j^k]_x,
\]

Infinitesimal rotation
Multilevel solve

- Recall block diagonal stiffness matrix

\[
L = \begin{pmatrix}
A^1 & 0 & \cdots & 0 \\
0 & B^1 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & 0
\end{pmatrix}
\]

- Therefore, each level can be solved independently

\[
A^q u^q = g^q
\]

\[
B^k w^k = W^k g^{k+1} \quad \text{for } q-1 \geq k \geq 1
\]

\[
A^1 v^1 = g^1
\]

- Decompose and solve in parallel
- Assemble solutions
- For coarse-graining

\[
u^q = \Phi^1, T v^1 + \sum_{k=1}^{q-1} \Psi_k, T w^k
\]
Homogenization accuracy
Resolve geometric nonlinearity

• Rotation-strain warping [Huang 2011]

\[ \hat{u}^q = \arg \min_u \int_{\Omega} \| \nabla u - \text{RS}(\nabla u^q) \|^2_F \]

s. t. \( S\hat{u}^q = 0 \)

• Cayley mapping to reduce over-estimation of rotation by \( \exp \)

\[ \text{Cay}(A) = (\mathbb{I}_{3\times3} - A/2)^{-1}(\mathbb{I}_{3\times3} + A/2) \]
Results
Comparisons

With [Nesme et al. 2009]
Element-wise diagonal matrix-valued basis functions

Both methods have only limited expressivity for complex anisotropic deformation.

With [Kharevych et al. 2009]
Regress elastic material tensor to encode anisotropy
Comparisons

With [Chen 2018]

(a) CR groundtruth  (b) our method  (c) [Chen et al. 2018]

Cannot handle aggressive coarsening well

Cannot adapt to boundary conditions
2D linear statics
3D linear dynamics

Fine:
# T: 20096
# V: 5120

Coarse:
# T: 2512
# V: 904
3D corotational dynamics

Fine:
# T: 20096
# V: 5120

Coarse:
# T: 2512
# V: 904
Complexity of precomputations

$O(n_q \log^{2d+1} n_q)$ \cite{Owhadi2017}
Stress homogenization

setting

composite material  fine (64 × 64)  coarse (1 × 1)
Structure analysis

\[ E(d) = 1/\text{div}(dd^T) : (A^1)^\dagger : \text{div}(dd^T) \]
Limitations and future work

• More accurate handling of geometric non-linearity
• Push the efficiency to the limit
• Extend to general nonlinear problem
  • Analytically adapt the basis functions, or
  • Numerically adapt the basis via fast update
• Combined with CHARMS framework for local adaptation
Thank you

Q&A

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