Numerical homogenization of multiscale problems

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Numerical homogenization of multiscale problem

Multiscale materials



Numerical homogenization of multiscale problem

Multiscale problems

We consider applications such as





▷ composite materials □ ▷ flow in a porous medium

that require numerical solution of partial differential equations with rough data (module of elasticity, conductivity, or permeability).

Major challenge: Features on multiple non-separated scales.

Elliptic problem: Homogenization and FEM

- Introduction to LOD
- High contrast data
- Applications
- Conclusions

Elliptic model problem

The Poisson equation

$$-\nabla \cdot \mathbf{A} \nabla u = f$$
 in Ω $u = 0$ on $\partial \Omega$

with data $0 < \alpha \le A \le \beta < \infty$ and $f \in L^2(\Omega)$.



Numerical homogenization of multiscale problem

Homogenization of an elliptic model problem

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with data $0 < \alpha \le A \le \beta < \infty$ and $f \in L^2(\Omega)$.

Homogenization theory Let $A = A(x/\epsilon)$ be ϵ -periodic, and consider

$$-\nabla \cdot (A(x/\epsilon)\nabla u_{\epsilon}(x,x/\epsilon)) = f(x).$$

It can be shown that as $\epsilon \to 0$, $u_{\epsilon} \to v$ solves

$$-\nabla\cdot(A^*\nabla v(x))=f(x),$$

- In 1D with no slow variation in A, $A^* = \frac{1}{\langle 1/A \rangle}$, i.e. the harmonic average.
- Otherwise A* is computed by solving a cell problem.

Homogenization of an elliptic model problem

The Poisson equation

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with data $0 < \alpha \le A \le \beta < \infty$ and $f \in L^2(\Omega)$.

Homogenization theory

- Requires $\epsilon \rightarrow 0$, i.e. very large scale separation.
- Requires periodic data.
- Complex geometry and boundary conditions are not covered by the theory.
- Numerical approaches inspired by homogenization theory (e.g. HMM and MsFEM) suffers form similar drawbacks.

Multiscale finite element method, (Hou & Wu), 1996. Heterogeneous multiscale method, (Engquist & E), 2003.

The Poisson equation (weak form): $u \in V = H_0^1(\Omega)$ such that

$$a(u, v) := \int_{\Omega} (\mathbf{A} \nabla u) \cdot \nabla v \, dx = \int_{\Omega} f \cdot v \, dx$$
 for all $v \in V$

with data $0 < \alpha \le A \le \beta < \infty$ and $f \in L^2(\Omega)$.

The Poisson equation (FE approximation): $u_h \in V_h \subset V$ such that

$$a(u_h, v) := \int_{\Omega} (\mathbf{A} \nabla u_h) \cdot \nabla v \, dx = \int_{\Omega} f \cdot v \, dx$$
 for all $v \in V_h$

with data $0 < \alpha \le A \le \beta < \infty$ and $f \in L^2(\Omega)$.

Numerical error (piecewise linear continuous FE approximation)

• For solution $u \in H^2(\Omega)$ we have

 $|||u - u_h||| := ||A^{1/2}\nabla(u - u_h)||_{L^2(\Omega)} \le C\beta^{1/2}h||D^2u||_{L^2(\Omega)} \sim C(\alpha, \beta, A')h.$

The mesh size *h* has to resolve the variations in *A*, e.g. *h* < *ϵ* if *A* is *ϵ*-periodic.

The Poisson equation (FE approximation): $u_h \in V_h \subset V$ such that

$$a(u_h, v) := \int_{\Omega} (\mathbf{A}
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with data $0 < \alpha \le A \le \beta < \infty$ and $f \in L^2(\Omega)$.

Example (periodic coefficient): $A(x) = 2 + \sin(2\pi x/\varepsilon), \varepsilon = 2^{-6}, f = 1$



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The Poisson equation (FE approximation): $u_h \in V_h \subset V$ such that

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New numerical approach

Objectives:

Find a subspace of V_H^{ms} ⊂ V_h for which the Galerkin approximation fulfills

$$|||u_h - u_H^{\mathsf{ms}}||| \le C(\alpha, \beta) H \approx C(\alpha, \beta, \mathbf{A'})h,$$

but with dim $(V_H^{ms}) \ll \dim(V_h)$.

- Show that a basis for V_{H}^{ms} can be constructed by local parallel computations.
- Demonstrate efficiency for applications where V_H^{ms} is reused (eigenvalue, time dependent, semi-linear, systems).

Variational multiscale method, (Hughes), 1995

Elliptic problem: Homogenization and FEM

Introduction to LOD

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Multiscale decomposition

- (coarse) FE mesh \mathcal{T} with parameter H > h
- P1-FE space $V_H := \{ v \in V \mid \forall T \in \mathcal{T}, v |_T \in P_1(T) \}$
- $\mathfrak{I}_{\mathcal{T}}: V \to V_H$ some interpolation operator



Decomposition

$$V = V_H \oplus V^f$$
 with $V^f := \text{kernel } \mathfrak{I}_{\mathcal{T}} = \{v \in V \mid \mathfrak{I}_{\mathcal{T}} v = 0\}$

Example:



rough coefficient

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2017-03-15 10/37

Multiscale decomposition

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Example:



Orthogonalization

• For each $v \in V$ define finescale projection $Qv \in V^{f}$ by

$$a(Qv,w) = a(v,w)$$
 for all $w \in V^{\mathsf{f}}$

a-Orthogonal Decomposition

$$V = V_H^{ms} \oplus V^{f}$$
 with $V_H^{ms} := (V_H - QV_H)$

Example:



Ideal multiscale representation

Given the space V_{H}^{ms} we construct a Galerkin approximation:

Ideal method Find $u_{H}^{ms} \in V_{H}^{ms}$ such that $a(u_{H}^{ms}, v) = (f, v), \ \forall v \in V_{H}^{ms}.$

We have that $u - u_H^{ms} = u_f \in V^f$ since u_H^{ms} is the *a*-orthogonal projection of *u* onto V_H^{ms} . Therefore

$$|||u_{f}|||^{2} = a(u, u_{f}) = (f, u_{f}) = (f, u_{f} - \Im_{\mathcal{T}} u_{f}) \leq \frac{C_{\Im_{\mathcal{T}}}}{\alpha^{1/2}} ||Hf||_{L^{2}(\Omega)} |||u_{f}|||.$$

For V_{H}^{ms} to be useful we need a discrete local basis.

Modified nodal basis

- ${\cal N}$ denotes set of interior vertices of ${\cal T}$
- $\phi_x \in V_H$ denotes classical nodal basis function ($x \in N$)
- $Q\phi_x \in V^{f}$ denotes the finescale correction of ϕ_x ($x \in N$)

Ideal multiscale FE space

$$V_H^{ms} = \operatorname{span} \{ \phi_x - Q \phi_x \mid x \in \mathcal{N} \}$$



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Modified nodal basis



2017-03-15 13 / 37

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Localization

• Define nodal patches of ℓ -th order $\omega_{T,\ell}$ about $T \in \mathcal{T}$





 $\omega_{T,1}$

 $\omega_{T,2}$

• Correctors $Q_{\ell}^{T}\phi_{x} \in V^{f}(\omega_{T,\ell}) := \{v \in V^{f} \mid v|_{\Omega \setminus \omega_{T,\ell}} = 0\}$ solve

$$a(Q_\ell^{\mathsf{T}}\phi_x,w) = \int_{\mathsf{T}} A
abla \phi_x \cdot
abla w \, dx \quad ext{for all } w \in V^{\mathsf{f}}(\omega_{\mathcal{T},\ell})$$

Localized multiscale FE spaces

$$V_{H,\ell}^{\mathsf{ms}} = \mathsf{span}\{\phi_x - \sum_{T \in \mathcal{T}} Q_\ell^T \phi_x \mid x \in \mathcal{N}\}$$

Fine scale discretization

• Finescale mesh





 \mathcal{T}_h with $h \leq H$

• Reference FE space

$$V_h := \{ v \in V \mid \forall T \in \mathcal{T}(\Omega), v |_T \in P_1(T) \}$$

mesh refinement

 \sim

• Reference FE solution $u_h \in V_h$ solves

$$a(u_h, v) = (f, v)$$
 for all $v \in V_h$

• Fully discrete correctors $Q_{\ell,h}^T \phi_x \in V_h^f(\omega_{T,\ell}) := V^f(\omega_{T,\ell}) \cap V_h$:

$$a(Q_{\ell,h}^{\mathsf{T}}\phi_x,w) = (A \nabla \phi_x, \nabla w)_{\mathsf{T}} \text{ for all } w \in V_h^{\mathsf{f}}(\omega_{\mathsf{T},\ell})$$

Localized Orthogonal Decomposition (LOD)

Fully discrete multiscale FE spaces

$$V_{H,\ell}^{\mathsf{ms},h} = \mathsf{span}\{\phi_x - \sum_{T \in \mathcal{T}} Q_{\ell,h}^T \phi_x \mid x \in \mathcal{N}\}$$

Fully discrete multiscale approximation $u_{H,\ell}^{ms,h} \in V_{H,\ell}^{ms,h}$

$$a(u_{H,\ell}^{{
m ms},h}, v) = (f,v) \quad ext{ for all } v \in V_{H,\ell}^{{
m ms},h}$$

Remarks:

• dim
$$V_{H,\ell}^{\mathsf{ms},h} = |\mathcal{N}| = \dim V_H$$

 The basis functions have local support, with overlap depending on *l*, and are independent.

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Lemma (Truncation error)

$$|||Q_h v_H - Q_{\ell,h} v_H||| \le C_1 \gamma^{\ell} |||Q_h v_H|||, \quad \forall v_h \in V_H$$

 $C_1 < \infty$ and $\gamma < 1$ depends on β/α but not A'.

By choosing $\ell = C_2 \log(H^{-1})$ with appropriate C_2 we guarantee that the truncation leads to a higher order perturbation:

Theorem (A priori error bound)

$$|||u_h - u_{H,\ell}^{\mathsf{ms},h}||| \le C(\alpha,\beta)H,$$

with C independent of A'.

M. & Peterseim, Localization of elliptic multiscale problems, 2014.

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Numerical experiment: Poisson's equation



Numerical experiment: Poisson's equation



Numerical experiment: Poisson's equation



3D implementation in python

- Trilinear shape functions on cubes.
- Petrov-Galerkin formulation reduces communication, Elfverson et.al. Numer. Math. 2016.
- Storage of all basis function is not needed. The full solution can be recomputed (at a lower cost) once ℑ_T u^{ms,h}_{Hℓ} is computed.



Corrector function $Q^T \phi_x$, implementation by Fredrik Hellman.

Numerical experiment: Poisson's equation 3D



Numerical experiment: Poisson's equation 3D



Numerical experiment: Poisson's equation 3D



Elliptic problem: Homogenization and FEM

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High contrast data

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High contrast data

Poisson equation:

$$-\nabla \cdot \mathbf{A} \nabla u = f$$
 in Ω $u = 0$ on $\partial \Omega$.

A = 1 in Ω_1 (black), $A = \alpha$ in Ω_{α} , $\alpha \ll 1$, and $f = \chi_{[1/4,3/4]^2}$.



- High contrast data with channels leads to non-local behaviour.
- The decay rate of the basis functions determines the accuracy of LOD.
- The choice of interpolant $\Im_{\mathcal{T}} v = \sum_{x \in \mathcal{N}} \bar{v}_{\omega_x} \phi_x$ affects the decay.

Numerical example: High contrast

High contrast data Three examples: $H = 2^{-4}$, $h = 2^{-10}$,



We let $\alpha = 10^{-1}, ..., 10^{-6}$ and plot $|||u_h - u_{H,k}^{ms,h}|||$ vs. *k*, with $\Im_{\mathcal{T}}^{SZ}$,



Numerical homogenization of multiscale problem

Scott-Zhang type interpolation

Nodal variables:

Let $x \in N$ be nodes of \mathcal{T} and $\sigma_x \subset \Omega$ associated domains. We define a $L^2(\sigma_x)$ -dual basis $\psi_x \in V_H$ fulfilling,

$$\int_{\sigma_x} \psi_x \phi_y = \delta_{xy}.$$

Let the nodal variable $N_x(v) = \int_{\sigma_x} \psi_x v$ and,

$$\mathfrak{I}^{\sigma}_{\mathcal{T}} v = \sum_{x \in \mathcal{N}} N_x(v) \phi_x.$$

- σ_x does not need to be full elements *T* or vertex patches $U_1(x)$.
- The stability of |N_x(v)| ≤ ||ψ||_{L²(σ_x)} ||v||_{L²(σ_x)} depends on the size and shape of σ_x and its distance to x.

Geometry dependent interpolation

Selection of σ_x :

By letting $\sigma_x \subset \Omega_1$ (frequently enough) we guarantee decay, i.e. nodes in high conductivity channels are needed.



Let $U_1(x)$ be the vertex patch at node x.

- Type I node: for x ∈ Ω₁ let σ_x ⊂ U₁(x) ∩ Ω₁, connected, and chosen so inf_{q∈ℝ} ||v − q||_{L²(σ_x)} ≤ CH||∇v||_{L²(σ_x)} holds (Poincaré).
- Type II node: for $x \in \Omega_{\alpha}$ let $\sigma_x = U_{\delta}(x)$, $0 < \delta \le 1$,

Weighted Poincaré inequality and decay

The following weighted Poincaré inequality holds:

$$\|\boldsymbol{A}^{1/2}\boldsymbol{v}_f\|_{L^2(\mathcal{T})} \leq CH \|\boldsymbol{A}^{1/2}\nabla\boldsymbol{v}_f\|_{L^2(U_1(\mathcal{T}))}, \quad \forall \boldsymbol{v}_f \in \boldsymbol{V}^{\mathrm{f}} = \mathsf{ker}(\mathfrak{I}_{\mathcal{T}}^{\sigma}).$$

This is used to prove contrast independent decay.

Theorem

With $\delta < 1/2$ we have,

$$\|\boldsymbol{A}^{1/2}\nabla \boldsymbol{Q}^{\mathsf{T}}\boldsymbol{v}_{\mathsf{H}}\|_{\Omega\setminus U_{k}(\mathsf{T})} \leq \boldsymbol{C}\gamma^{k}\|\boldsymbol{A}^{1/2}\nabla \boldsymbol{Q}^{\mathsf{T}}\boldsymbol{v}_{\mathsf{H}}\|_{L^{2}(\Omega)},$$

where C and γ are independent of β/α .

Hellman & M. Contrast independent localization of multiscale problems, arXiv

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We let $\alpha = 10^{-1}, \ldots, 10^{-6}$ and plot $|||u_h - u_{H,k}^{\text{ms},h}|||$ vs. k with $\mathfrak{I}_{\mathcal{T}}^{\sigma}$,



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Prototypical self-adjoint eigenvalue problem

$$-\nabla \cdot \mathbf{A} \nabla u = \lambda u$$
 in Ω $u = 0$ on $\partial \Omega$

with data $0 < \alpha \le A \le \beta < \infty$



Prototypical self-adjoint eigenvalue problem (variational form): find $u \in V := H_0^1(\Omega)$ and $\lambda \in \mathbb{R}$ such that

$$a(u,v) := \int_{\Omega} (A \nabla u) \cdot \nabla v \, dx = \lambda \int_{\Omega} u \cdot v \, dx$$
 for all $v \in V$

with data $0 < \alpha \le A \le \beta < \infty$



Prototypical self-adjoint eigenvalue problem (FE approximation): $u_h \in V_h \subset V$ and $\lambda_h \in \mathbb{R}$ such that

$$a(u_h, v) := \int_{\Omega} (\mathbf{A} \nabla u_h) \cdot \nabla v \, dx = \lambda_h \int_{\Omega} u_h \cdot v \, dx \text{ for all } v \in V_h$$

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with data $0 < \alpha \le A \le \beta < \infty$

Numerical error (piecewise linear continuous FE approximation)

• For an eigenpair $(u^{(k)}, \lambda^{(k)})$ with $u^{(k)} \subset H^2(\Omega)$ it holds

$$\begin{split} \lambda^{(k)} &\leq \lambda_h^{(k)} \leq \lambda^{(k)} + C(\alpha, \beta, A', k)h^2, \\ \| \| u^{(k)} - u_h^{(k)} \| \| &:= \| A^{1/2} \nabla (u^{(k)} - u_h^{(k)}) \|_{L^2(\Omega)} \leq C(\alpha, \beta, A', k)h. \end{split}$$

The mesh size *h* has to resolve the variations in *A*, e.g. *h* < *ϵ* if *A* is periodic.

LOD approximation

LOD: Find
$$u_{H,\ell}^{\text{ms},h} \in V_{H,\ell}^{\text{ms},h}$$
, $\lambda_{H,\ell}^{\text{ms},h} \in \mathbb{R}$
 $a(u_{H,\ell}^{\text{ms},h}, v) = \lambda_{H,\ell}^{\text{ms},h}(u_{H,\ell}^{\text{ms},h}, v) \text{ for all } v \in V_{H,\ell}^{\text{ms},h}$

Theorem

$$\begin{split} \lambda_h^{(k)} &\leq \lambda_{H,\ell}^{\text{ms},h,(k)} \leq \lambda_h^{(k)} + CH^4, \\ &|||u_h^{(k)} - u_{H,\ell}^{\text{ms},h,(k)}||| \leq CH^2, \end{split}$$

with C independent of A' and the regularity of the eigenfunctions and (λ_h, u_h) is the reference solution.

M. & Peterseim, Computation of eigenvalues by nume. upscaling, 2015.

Numerical example: eigenvalues



k	$\lambda_h^{(k)}$	$e^{(k)}(1/2\sqrt{2})$	$e^{(k)}(1/4\sqrt{2})$	$e^{(k)}(1/8\sqrt{2})$	$e^{(k)}(1/16\sqrt{2})$
1	21.4144522	5.472755371	0.237181706	0.010328293	0.000781683
2	40.9134676	-	0.649080539	0.032761482	0.002447049
3	44.1561133	-	1.687388874	0.097540102	0.004131422
4	60.8278691	-	1.648439518	0.028076168	0.002079812
5	65.6962136	-	2.071005692	0.247424446	0.006569640
6	70.1273082	-	4.265936007	0.232458016	0.016551520
7	82.2960238	-	3.632888104	0.355050163	0.013987920
8	92.8677605	-	6.850048057	0.377881216	0.049841235
9	99.6061234	-	10.305084010	0.469770376	0.026027378
10	109.1543283	-	-	0.476741452	0.005606426
11	129.3741945	-	-	0.505888044	0.062382302
12	138.2164330	-	-	0.554736550	0.039487317
13	141.5464639	-	-	0.540480876	0.043935515
14	145.7469718	-	-	0.765411709	0.034249528
15	152.6283573	-	-	0.712383825	0.024716759
16	155.2965039	-	-	0.761104705	0.026228034
17	158.2610708	-	-	0.749058367	0.091826207
18	164.1452194	-	-	0.840736127	0.118353184
19	171.1756923	-	-	0.946719951	0.111314058
20	179.3917590	-	-	0.928617606	0.119627862

Table: Errors
$$e^{(k)}(H) =: \frac{\lambda_{H}^{ms,(k)} - \lambda_{h}^{(k)}}{\lambda_{h}^{(k)}}$$
 and $h = 2^{-7} \sqrt{2}$.

Parabolic equations

The parabolic problem: Find $u \in V$ such that

$$(\dot{u}, v) + (A \nabla u, \nabla v) = (f(t), v), \quad \forall v \in V, \quad t > 0$$

and $u(0) = u_0 \in L^2(\Omega)$. We assume A to be independent of t. FE Backward Euler: Find $u_h^n \in V_h$ such that

$$(\bar{\partial}_t u_h^n, v) + a(u_h^n, v) = (f^n, v), \quad \forall v \in V_h,$$

and $u_h^0 \in V_h$ some approximation of u_0 .

LOD: Find $(u_H^{ms})^n \in V_{H,\ell}^{ms,h}$ such that $(\overline{\partial}_t (u_H^{ms})^n, v) + a((u_H^{ms})^n, v) = (f^n, v), \quad \forall v \in V_{H,\ell}^{ms,h},$ and $(u_H^{ms})^0 \in V_{H,\ell}^{ms,h}$ some approximation of u_0 .

Parabolic equations

Theorem

$$\|u_{h}^{n}-(u_{H}^{ms})^{n}\|_{L^{2}(\Omega)} \leq C(1+\log(\frac{t_{n}}{\tau}))H^{2}(t_{n}^{-1}\|u_{h}^{0}\|_{L^{2}(\Omega)}+\|f\|_{W^{1,\infty}(L^{2}(\Omega)})$$

with C independent of A'.

- The analysis uses classic a priori error estimation techniques and the elliptic results.
- The term t_n⁻¹ appears also in u − u_h bounds if u₀ ∈ L²(Ω). The log term can be avoided if f(t) ∈ H₀¹(Ω).
- The case f = f(u) can also be treated, under certain growth conditions on f'(u) and f''(u).
- The case A = A(t) or A = A(u) is not covered and would require updates of V^{ms,h}_{H,l}.

Numerical experiment: The heat equation



M.& Persson, *Multiscale techniques for parabolic problems,* arXiv 1504.08140.

More applications

Stationary/eigenvalue problems

- Semilinear, (Henning, M., Peterseim), 2014.
- Gross-Pitaevskii, (Henning, M., Peterseim), 2014.
- Helmholtz, (Gallistl & Peterseim), 2015.
- Reduced basis, (Abdulle & Henning), 2015.
- Elasticity, (Henning & Persson), 2016.
- High contrast, (Peterseim & Scheichl), 2016.
- Helmholtz, (Ohlberger & Verfürth), 2017.
- Iterative solvers, (Kornhuber & Yserentant), 2017.

Time-dependent problems

- Thermoelasticity, (M. & Persson), 2017.
- Wave equation, (Abdulle & Henning), 2017.
- Two phase flow, (Hellman & M.), ongoing

- Elliptic problem: Homogenization and FEM
- Introduction to LOD
- High contrast data
- Applications
- Conclusions

- By LOD we compute an effective stiffness matrix on a coarse scale. (numerical homogenization)
- Rapidly varying diffusion of low contrast is well understood.
- Recent development in high contrast problems which is a great challenge for any method.
- Great reduction in computational cost when the basis is reused (load cases, eigenvalues, time dependent, non-linear, control).
- Future challenges: random diffusion, quasi-linear problems, efficient implementation, nearly periodic problems.

Thank you for your attention!