Analysis of multiscale methods

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Multiscale problems

Applications such as





▷ composite materials □ ▷ flow in a porous medium

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

Major challenge: Features on multiple non-separated scales.

Finite elements (FE) – methodology

The numerical solution of PDEs by FEM consists of

- construction of an "appropriate" FE mesh
- choosing (local) basis functions (of variable degree of approximation)

An optimal construction should be adapted to the local behavior of the exact solution and, hence, should take into account

- local singularities of the solution (e.g. singularities at re-entrant corners)
- effects of singular perturbations in the solutions (e.g. boundary layers)
- scales and amplitudes of rough coefficients







Setting and Motivation

- Multiscale Method and Convergence
- Full Discretization and Numerical Experiments
- Application to Other Problems
- Conclusion

Poisson's equation

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

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



Poisson's equation (variational form): $u \in V := H_0^1(\Omega)$ s.t.

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

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



oscillatory coefficient

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Examples (periodic coefficients)

- We have $|||u u_h||| := ||A^{1/2}\nabla(u u_h)|| \le C(A, f)h = C'(f)\frac{h}{\epsilon}$.
- We need to resolve the fine scale features even to get the coarse scale behavior right.

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

Examples (rough coefficients)



Objectives

Without any assumptions on scales ...

- Construction of an upscaled variational problem based on a generalized FEM (coarse mesh T of size H & modified nodal basis functions)
- Computation of basis functions involves solution of PDE only on local patches of coarse elements with diam ≈ H log(1/H)
- Error estimate

$$|||u - u_H^{ms}||| := ||A^{1/2}\nabla(u - u_H^{ms})|| \le C(f)H$$

with C(f) independent of scales of A

A. Målqvist and D. Peterseim.

Localization of Elliptic Multiscale Problems.

ArXiv e-prints, Oct. 2011.

Some known methods

- Upscaling techniques: Durlofsky et al. 98, Iliev et al. 08
- Variational multiscale method: Hughes et al. 95, Arbogast 04, Larson-Målqvist 05, Nolen et al. 08
- Multiscale FEM: Hou-Wu 96, Efendiev-Ginting 04, Aarnes-Lie 06
- Residual free bubbles: Brezzi et al. 98
- Multiscale finite volume method: Jenny et al. 03
- Heterogeneous multiscale method: Engquist-E 03, E-Ming-Zhang 04, Ohlberger 05
- Equation free: Kevrekidis et al. 05
- Metric based upscaling: Owhadi et al. 06
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Common idea

Local approximations (in parallel) on a fine scale are used to modify a coarse scale space or equation

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Remark

Error analysis rely on strong assumptions such as scale separation and periodicity

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Multiscale decomposition

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



Orthogonalization

• For each $v \in V_H$ define finescale projection $\mathfrak{F} v \in V^{\mathsf{f}}$ by

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

Orthogonal Decomposition

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

Example:



Error analysis

Lemma

$$|||u - u_H^{ms}||| \le C_{ol} C_{\Im_T} \alpha^{-1/2} ||Hf||_{L^2(\Omega)}$$

Sketch of proof:

- recall $\|v \Im_{\mathcal{T}} v\|_{L^{2}(T)} \leq C_{\Im_{\mathcal{T}}} H \|\nabla v\|_{L^{2}(\omega_{T})}$ with $\omega_{\mathcal{T}} := \bigcup \{K \in \mathcal{T} \mid T \cap K \neq \emptyset\}$ [Carstensen/Verfürth '99]
- orthogonal decomposition yields $u^{f} := u u_{H}^{ms} \in V^{f}$
- ℑ_T u^f = 0, interpolation error estimate, and finite overlap of the patches ω_T conclude the proof

$$|||u^{f}|||^{2} = a(\underbrace{u^{f} + u^{ms}_{H}}_{=u}, u^{f}) = F(u^{f}) = F(u^{f} - \mathfrak{I}_{T}u^{f})$$

$$\leq \sum_{T \in \mathcal{T}} ||f||_{L^{2}(T)} ||u^{f} - \mathfrak{I}_{T}u^{f}||_{L^{2}(T)} \leq C_{ol}C_{\mathfrak{I}_{T}}\alpha^{-1/2} ||Hf||_{L^{2}(\Omega)} |||u^{f}||| \square$$

Modified nodal basis

- ${\cal N}$ denotes set of interior vertices of ${\cal T}$
- $\lambda_x \in V_H$ denotes classical nodal basis function ($x \in N$)
- $\phi_x = \Im \lambda_x \in V^{\mathsf{f}}$ denotes finescale correction of $\lambda_x \ (x \in \mathcal{N})$

Ideal multiscale FE space

$$\mathcal{I}_{H}^{\mathsf{ms}} = \mathsf{span}\left\{\lambda_{x} - \phi_{x} \mid x \in \mathcal{N}\right\}$$



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Modified nodal basis



Assumpting more reglarity on A we have $\lambda_x - \phi_x \in H^2(\Omega) \cap H^1(\Omega)$.

Localization

• Define nodal patches of *k*-th order $\omega_{x,k}$ about $x \in N$



Localized corrections φ_{x,k} ∈ V^f(ω_{x,k}) := {v ∈ V^f | v|_{Ω\ω_{x,k}} = 0} solve

$$a(\phi_{x,k}, w) = a(\lambda_x, w)$$
 for all $w \in V^{\mathsf{f}}(\omega_{x,k})$

Localized multiscale FE spaces

$$V_{H,k}^{ms} = \operatorname{span}\{\lambda_x - \phi_{x,k} \mid x \in \mathcal{N}\}$$

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Multiscale approximation seeks $u_{H,k}^{ms} \in V_{H,k}^{ms}$ such that $a(u_{H,k}^{ms}, v) = F(v)$ for all $v \in V_{H,k}^{ms}$

Remarks:

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

- basis functions of the multiscale method have local support and are totally independent
- overlap of the supports is proportional to the parameter *k*
- error analysis suggests $k \approx \log \frac{1}{H}$
- method can take advantage of periodicity

Lemma (Truncation error)

There exist $C_1 < \infty$ and $\gamma < 1$ independent of x, k, H such that

 $|||\phi_x - \phi_{x,k}||| \le C_1 \gamma^k |||\phi_x|||.$

Sketch of proof:

- Let $\zeta_{k,\ell} = \begin{cases} 0, & \text{in } \omega_{x,k-\ell} \\ 1, & \text{in } \Omega \setminus \omega_{x,k} \end{cases}$ be a cut off function.
- Since $(1 \zeta_{k,1})\phi_x \in V^{\mathsf{f}}(\omega_k)$ we have $\||\phi_x - \phi_{x,k}\|| \leq \||\phi_x - (1 - \zeta_{k,1})\phi_x\|| \leq \|\zeta_{k,1}\|_{L^{\infty}(\Omega)} \||\phi_x\||_{\Omega \setminus \omega_{x,k-1}} + \|\nabla \zeta_{x,k}\|_{L^{\infty}(\Omega)} \|\phi_x - \Im_{\mathcal{T}}\phi_x\|_{L^2(\Omega \setminus \omega_{x,k-1})} \leq \||\phi_x\||_{\Omega \setminus \omega_{x,k-1}}.$
- We have $\||\phi_x\||_{\Omega\setminus\omega_{x,k}}^2 \leq (A\zeta_{k,\ell}^2\nabla\phi_x,\nabla\phi_x) = (A\nabla\phi_x,\nabla(\zeta_{k,\ell}^2\phi_x)) 2(A\zeta_{k,\ell}(\phi_x \Im_{\mathcal{T}}\phi_x)\nabla\zeta_{k,\ell},\nabla\phi_x) \leq \ell^{-1} \||\phi_x\||_{\Omega\setminus\omega_{x,k-\ell}}^2.$
- Repeat $\||\phi_x||_{\Omega\setminus\omega_{x,\ell^k}}^2 \lesssim (C_2/\ell)^k \||\phi_x||^2 := \gamma^k \||\phi_x|\|^2$, where C_2 depends on the contrast in A.

Error Analysis

Theorem (Main result)

$$|||u - u_{H,k}^{\mathsf{ms}}||| \le C_2 \left(k^d ||H^{-1}||_{L^{\infty}(\Omega)} \gamma^k ||f||_{L^2(\Omega)} + ||Hf||_{L^2(\Omega)} \right)$$

holds with a constant C_2 that does not depend on H, k, f, or u.

Sketch of proof:

- Let $\tilde{u}_{H,k}^{\text{ms}} = \sum_{x \in \mathcal{N}} u_H^{\text{ms}}(x) (\lambda_x \phi_{x,k})$ and note $|||u u_{H,k}^{\text{ms}}|||^2 \le |||u \tilde{u}_{H,k}^{\text{ms}}|||^2$ since $u_{H,k}^{\text{ms}}$ is a projection.
- We split the error $u \tilde{u}_{H,k}^{ms} = (u u_H^{ms}) + (u_H^{ms} \tilde{u}_{H,k}^{ms})$ and note $|||u u_H^{ms}||| \leq ||Hf||_{L^2(\Omega)}$ using previous Lemma.
- Finally $|||u_{H}^{ms} \tilde{u}_{H,k}^{ms}|||^{2} \leq \sum_{x \in \mathcal{N}} u_{H}^{ms}(x)^{2} |||\phi_{x} \phi_{x,k}|||^{2} \leq \sum_{x \in \mathcal{N}} u_{H}^{ms}(x)^{2} \gamma^{2k} ||\phi_{x}||^{2} \leq k^{2d} ||H^{-1}||_{L^{\infty}(\Omega)}^{2} \gamma^{2k} ||f||_{L^{2}(\Omega)}^{2}.$

Error Analysis

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Theorem holds without any assumptions on scales or regularity!

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Full Discretization and Numerical Experiments

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Full 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 corrections φ^h_{x,k} ∈ V^f_h(ω_{x,k}) := V^f(ω_{x,k}) ∩ V_h satisfy
 a(φ^h_{x,k}, w) = a(λ_x, w) for all w ∈ V^f_h(ω_{x,k})

Full discretization

Fully discrete multiscale FE spaces

$$V_{H,k}^{\mathrm{ms},h} = \mathrm{span}\{\lambda_x - \phi_{x,k}^h \mid x \in \mathcal{N}\}$$

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

$$a(u_{H,k}^{\mathrm{ms},h},v)=F(v) \quad ext{ for all } v\in V_{H,k}^{\mathrm{ms},h}$$

Theorem (Error estimate)

 $|||u - u_{H,k}^{\mathsf{ms},h}||| \le C_3 \left(|||u - u_h||| + k^d ||H^{-1}||_{L^{\infty}(\Omega)} \gamma^k ||f||_{L^2(\Omega)} + ||Hf||_{L^2(\Omega)} \right)$

holds with a constant C_3 that does not depend on H, h, k, f, or u.

Numerical experiment I



Numerical experiment I



Numerical experiment I



Numerical experiment II



Numerical experiment II



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Numerical experiment II



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Semi-linear PDE's

Let $u \in V$ solve,

$$-\nabla \cdot A \nabla u + F(u, \nabla u) = g$$
, in Ω $u = 0$ on $\partial \Omega$,

where $0 < \alpha \le A \le \beta$, *F* is monotone and Lipschitz continuous in both arguments (L_1 , L_2 of same size or less than β). Let

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

as before (i.e. only depending on A not F).



P. Henning, A. Målqvist, and D. Peterseim.

A rigorous multiscale method for semi-linear elliptic problems.

ArXiv e-prints, Nov. 2012.

Semi-linear PDE's

Error bound

Let u_h be the finite element reference solution on a fine mesh.

Lemma

 $\|\nabla(u_h - u_H^{\mathsf{ms},h})\|_{L^2(\Omega)} \lesssim \|Hf\|_{L^2(\Omega)} + H(L_1 + L_2)\|f\|_{H^{-1}(\Omega)}$

- Same basis functions are used i.e. same decay rate.
- A bound for $u_{H,k}^{ms,h}$ follows using monotonicity and similar arguments as in the linear case.
- The basis will not change in the non-linear iteration.

Eigenvalue Problems

Let $u \in V$ and $\lambda \in \mathbf{R}$ solve,

$$-\nabla \cdot A \nabla u = \lambda u$$
, in Ω $u = 0$ on $\partial \Omega$.

We use the same space V_{H}^{ms} and solve,

$$a(u_H^{\mathrm{ms}}, v) = \lambda_H(u_H^{\mathrm{ms}}, v),$$

for all $v \in V_H^{ms}$. We let $\mathfrak{T}_{\mathcal{T}}$ be the modified Clement interpolant defined by $(\mathfrak{T}_{\mathcal{T}}v)(x) = \int_{\Omega} \lambda_x v \, dx / \int_{\Omega} \lambda_x \, dx$, $\mathfrak{T}_{\mathcal{T}}v = \sum_{x \in \mathcal{N}} (\mathfrak{T}_{\mathcal{T}}v)(x) \lambda_x$. Note that u_H^{ms} is *a*-orthogonal and almost L^2 -orthogonal to V^f since,

$$(u_H^{\mathrm{ms}}, v_f) = (u_H^{\mathrm{ms}} - \mathfrak{I}_{\mathcal{T}} u_H^{\mathrm{ms}}, v_f - \mathfrak{I}_{\mathcal{T}} v_f) \leq H^2 \|A^{1/2} \nabla u_H^{\mathrm{ms}}\|_{L^2(\Omega)} \|A^{1/2} \nabla v_f\|_{L^2(\Omega)},$$

since $(\lambda_x, v_f) = 0$ by the definition of $V^f = \{v \in V : \mathfrak{I}_T v = 0\}$.

Eigenvalue Problems

Lemma

For
$$H \leq \ell^{-1/4} \alpha^{1/2} (\lambda_h^{(\ell)})^{-1/2}$$
 it holds, $\frac{\lambda_h^{(\ell)} - \lambda_H^{(\ell)}}{\lambda_h^{(\ell)}} \leq \ell^{1/2} (\lambda_h^{(\ell)})^2 \alpha^{-2} H^4.$

We get very rapid convergence for the lowest eigenvalues using approximations in the space V_{H}^{ms} .

- A very coarse *H* can be used: *H^{−d}* basis functions has to be computed on patches of size *H* · *log*(*H*).
- A coarse (H^{-d}) eigenvalue problem then has to be solved in order to approximate the H^{-d} smallest eigenvalues
 The choice of interpolation operator when constructing

$$V^{\mathsf{f}} = \{ v \in V : \mathfrak{I}_{\mathcal{T}} v = 0 \}$$
 is crucial.

A. Målqvist and D. Peterseim.

Computation of eigenvalues by numerical upscaling. ArXiv e-prints, Dec. 2012.

Eigenvalue Problem



l	$\lambda_h^{(\ell)}$	$e^{(\ell)}(1/2\sqrt{2})$	$e^{(\ell)}(1/4\sqrt{2})$	$e^{(\ell)}(1/8\sqrt{2})$	$e^{(\ell)}(1/16\sqrt{2})$
1	9.6436869	0.003494567	0.000034466	0.000000546	0.000000010
2	15.1989274	0.009621397	0.000079887	0.00000845	0.00000010
3	19.7421815	0.023813222	0.000213097	0.000002073	0.00000023
4	29.5281571	0.096910157	0.000724615	0.000006574	0.00000076
5	31.9265496	0.094454625	0.000874659	0.000009627	0.00000138
6	41.4922250	-	0.002395227	0.000019934	0.00000254
7	44.9604884	-	0.002443271	0.000019683	0.00000223
8	49.3631826	-	0.003651870	0.000028869	0.00000308
9	49.3655623	-	0.004266472	0.000032835	0.00000355
10	56.7389993	-	0.006863742	0.000055219	0.00000618
11	65.4085991	-	0.011534878	0.000082414	0.00000856
12	71.0947630	-	0.012596114	0.000090083	0.000001002
13	71.6064671	-	0.014249938	0.000098736	0.000001006
14	79.0043994	-	0.021801461	0.000164436	0.000001605
15	89.3706421	-	0.033550079	0.000211985	0.000002296
16	92.3648207	-	0.040060692	0.000239441	0.000002295
17	97.4459210	-	0.037438984	0.000284936	0.000002724
18	98.7545147	-	0.044544409	0.000269854	0.000002559
19	98.7545639	-	0.047835987	0.000276139	0.000002539
20	101.6755971		0.038203654	0.000297356	0.000002909

Table : Errors
$$e^{(\ell)}(H) =: \frac{\lambda_H^{(\ell)} - \lambda_h^{(\ell)}}{\lambda_h^{(\ell)}}$$
 and $h = 2^{-7} \sqrt{2}$.

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Eigenvalue Problem



l	$\lambda_{h}^{(\ell)}$	$e^{(\ell)}(1/2\sqrt{2})$	$e^{(\ell)}(1/4\sqrt{2})$	e ^(ℓ) (1/8 √2)	e ^(ℓ) (1/16 √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
$$e^{(\ell)}(H) =: \frac{\lambda_H^{(\ell)} - \lambda_h^{(\ell)}}{\lambda_h^{(\ell)}}$$
 and $h = 2^{-7}\sqrt{2}$.

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- Setting and Motivation
- Multiscale Method and Convergence
- Full discretization and Numerical Experiments
- Application to Other Problems
- Conclusion

Conclusion

- A variational multiscale FEM that yields scale-independent textbook convergence and, hence, leads to reliable computational approximation of multiscale problems.
- Numerical experiments confirms the theoretical results but shows less sensitive to high contrast than theory suggests.
- The basis functions are useful for other equations e.g. semi-linear problems and eigenvalue problems.