Localized Orthogonal Decomposition techniques for solving multiscale problems

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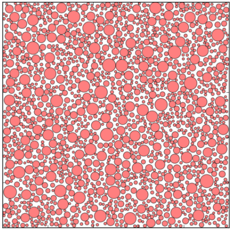
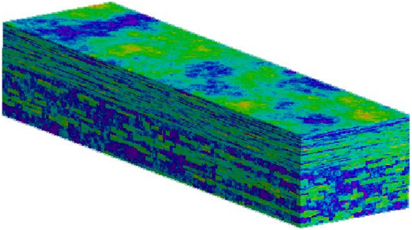
Multiscale problems

Applications such as



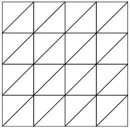


▹ composite materials ▹ flow in a porous medium

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

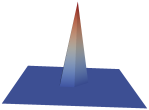
Major challenge: Features on multiple non-separated scales.

Finite elements (FE) – methodology

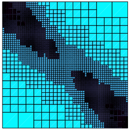


The numerical solution of PDEs by FEM consists of

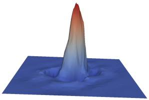
- construction of an "appropriate" FE mesh
- choosing (local) basis functions (of variable degree of approximation)



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



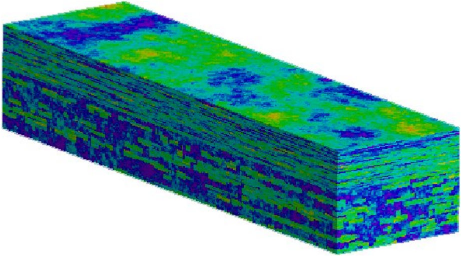
Outline

Model multiscale problem

Poisson's equation

$$-\nabla \cdot A \nabla u = f \quad \text{in } \Omega \qquad u = 0 \quad \text{on } \partial\Omega$$

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



Model multiscale problem

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

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

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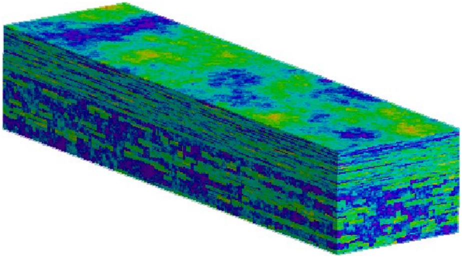

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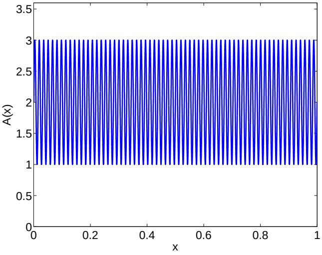
Example (periodic coefficient): $A(x) = 2 + \sin(2\pi x/\varepsilon)$, $\varepsilon = 2^{-6}$, $f = 1$



oscillatory coefficient

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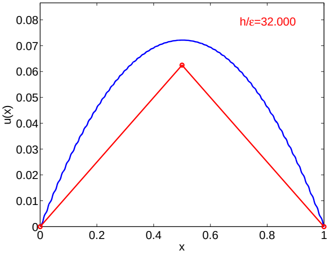
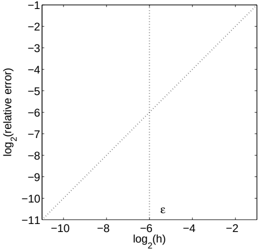


solution and P1-FEM-approximation



$\log_2(H^1(\Omega)-\text{error})$ vs. $\log_2(h)$

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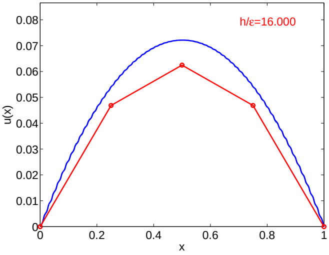

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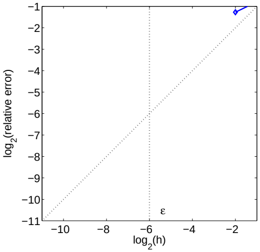

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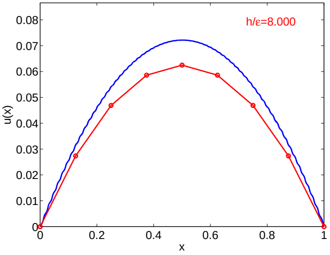

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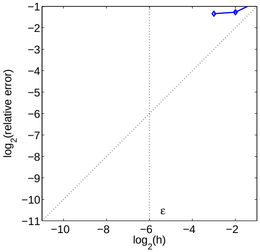

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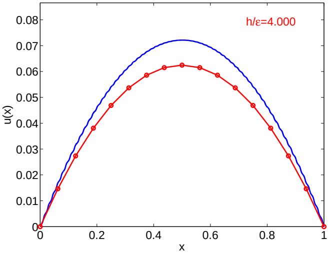

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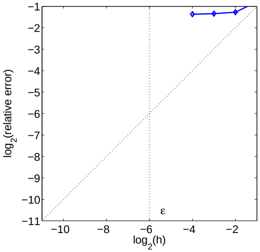

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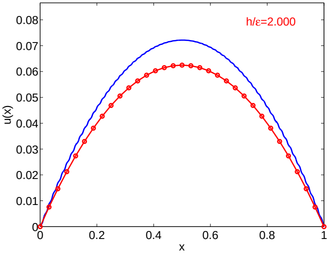

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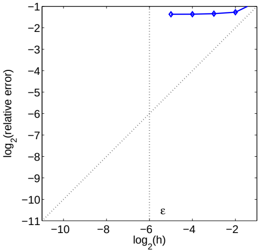

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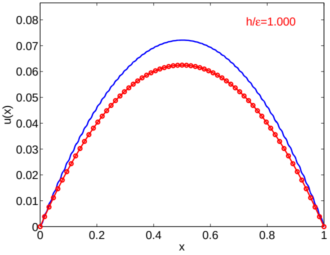

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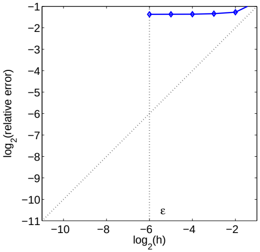

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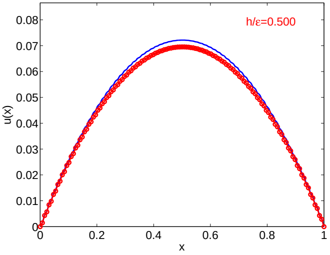

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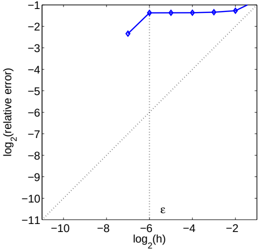

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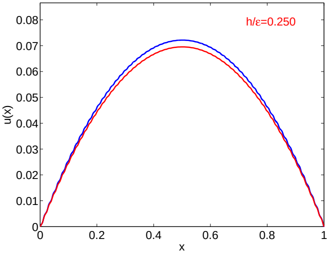

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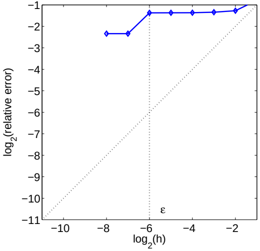

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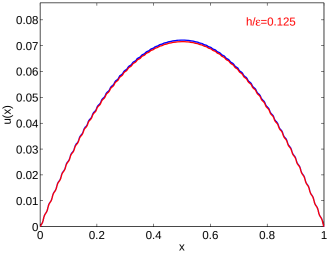

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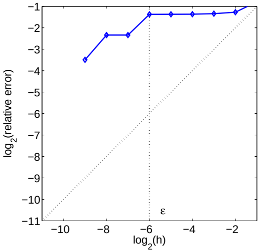

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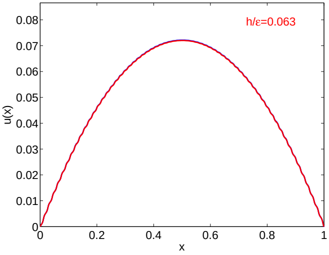

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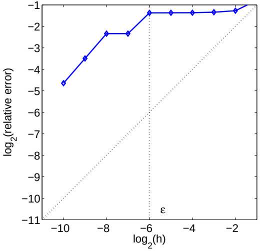

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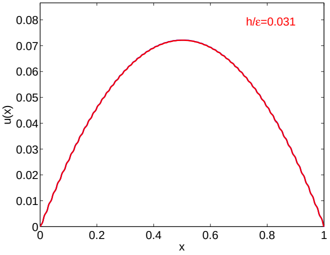

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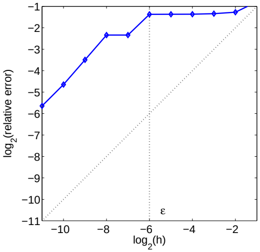

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Examples (periodic coefficients)

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

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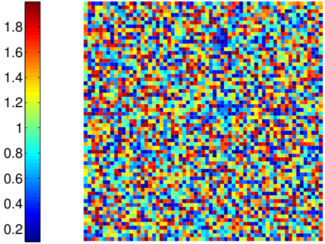
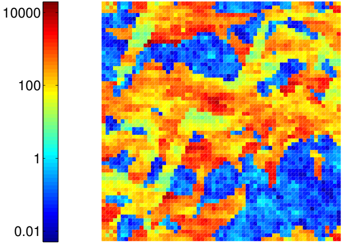
Examples (rough coefficients)



random material (academic)



porous medium (SPE10 benchmark)

Objectives

Without any assumptions on scales ...

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

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

with $C(f)$ independent of scales of A

A. Målqvist and D. Peterseim.
Localization of Elliptic Multiscale Problems.
Mathematics of Computation, 2014.

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, Larsson et al. 10
- 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
- ...

Common idea

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

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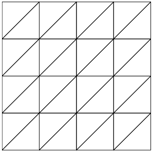
Remark

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

Outline

Multiscale decomposition

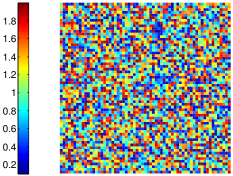
- (coarse) FE mesh $\mathcal{T}$ with parameter H
- P1-FE space $V_H := \{v \in V \mid \forall T \in \mathcal{T}, v|_T \in P_1(T)\}$
- $\mathfrak{I}_{\mathcal{T}} : V \to V_H$ quasi-interpolation operator



Decomposition

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

Example:



rough coefficient

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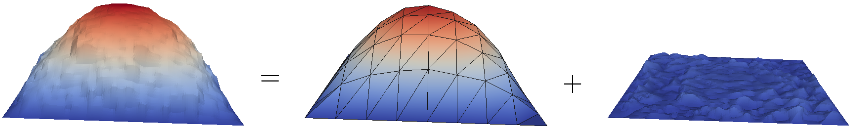


$u \in V$ $\qquad$ $u_H \in V_H$ $\qquad$ $u^{\mathrm{f}} \in V^{\mathrm{f}}$

Orthogonal decomposition

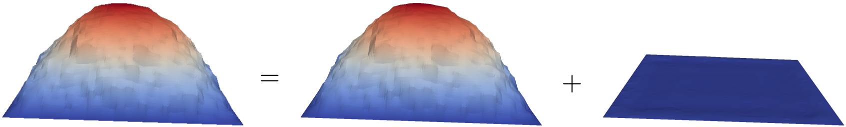
- For each $v \in V_H$ define finescale projection $\mathfrak{F}v \in V^{\mathrm{f}}$ by

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

Orthogonal Decomposition

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

Example:



$u \in V \quad = \quad u_H^{\mathrm{ms}} \in V_H^{\mathrm{ms}} \quad + \quad u^{\mathrm{f}} \in V^{\mathrm{f}}$

Error analysis

Lemma

$$|||u - u_H^{\mathrm{ms}}||| \leq C\alpha^{-1/2}||Hf||_{L^2(\Omega)}$$

Sketch of proof:

- Orthogonal decomposition yields $u^{\mathrm{f}} := u - u_H^{\mathrm{ms}} \in V^{\mathrm{f}}$
- We use that $\mathfrak{I}_{\mathcal{T}} u^{\mathrm{f}} = 0$ and an interpolation estimate to get,

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

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

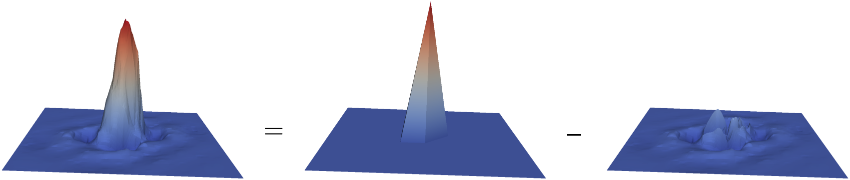
Modified nodal basis

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

Ideal multiscale FE space

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

Example



$\lambda_x - \phi_x \in V_H^{\mathrm{ms}}$ = $\lambda_x \in V_H$ − $\phi_x \in V^{\mathrm{f}}$

Modified nodal basis

- $\mathcal{N}$ denotes set of interior vertices of $\mathcal{T}$
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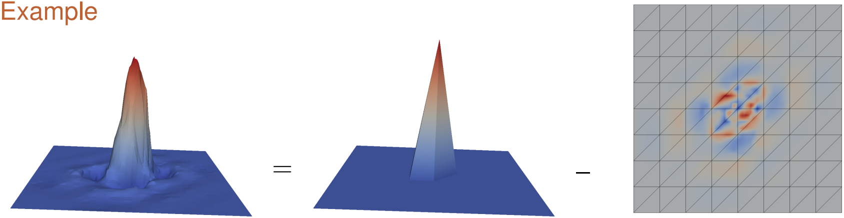
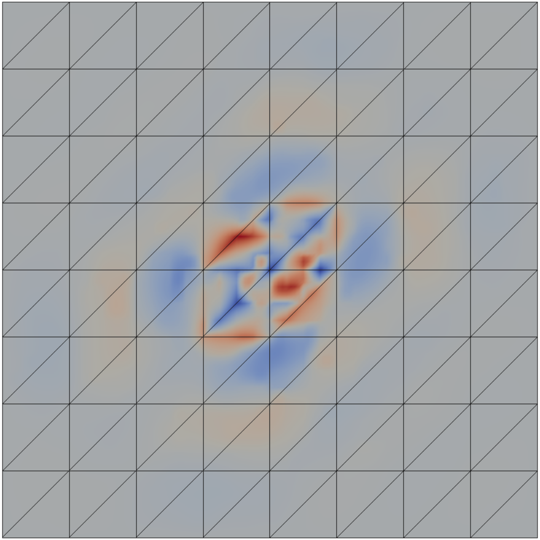
$$V_H^{\mathrm{ms}} = \mathrm{span}\,\{\lambda_x - \phi_x \mid x \in \mathcal{N}\}$$

Example



$\lambda_x - \phi_x \in V_H^{\mathrm{ms}}$ $\quad=\quad$ $\lambda_x \in V_H$ $\quad-\quad$ $\phi_x \in V^{\mathrm{f}}$

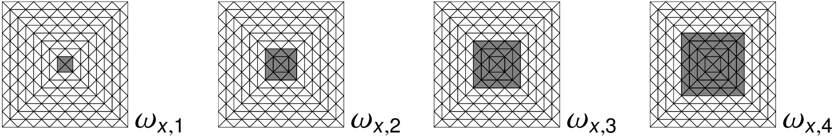
Modified nodal basis



Assumping more reglarity on A we have $\lambda_x - \phi_x \in H^2(\Omega) \cap H^1_0(\Omega)$.

Localization

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



- Localized corrections $\phi_{x,k} \in V^{\mathrm{f}}(\omega_{x,k}) := \{v \in V^{\mathrm{f}} \mid v|_{\Omega\setminus\omega_{x,k}} = 0\}$ solve

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

Localized multiscale FE spaces

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

The multiscale method

Multiscale approximation seeks $u^{\text{ms}}_{H,k} \in V^{\text{ms}}_{H,k}$ such that

$$a(u^{\text{ms}}_{H,k}, v) = F(v) \quad \text{for all } v \in V^{\text{ms}}_{H,k}$$

Remarks:

- $\dim V^{\text{ms}}_{H,k} = |\mathcal{N}| = \dim V_H$
- 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

Error Analysis

Lemma (Truncation error)

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

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

Theorem (Main result)

$$|||u - u^{\mathrm{ms}}_{H,k}||| \leq C_2 \left(\gamma^k \|f\|_{L^2(\Omega)} + \|Hf\|_{L^2(\Omega)} \right)$$

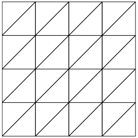
holds with a constant C_2 that does not depend on H, f, or u.

The Theorem holds without any assumptions on scales or regularity!

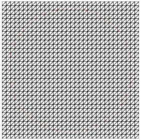
Outline

Full discretization

- Finescale mesh



mesh refinement



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

- Reference FE space

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

- Reference FE solution $u_h \in V_h$ solves

$$a(u_h, v) = F(v) \quad \text{for all } v \in V_h$$

- Fully discrete corrections $\phi^h_{x,k} \in V^{\mathrm{f}}_h(\omega_{x,k}) := V^{\mathrm{f}}(\omega_{x,k}) \cap V_h$ satisfy

$$a(\phi^h_{x,k}, w) = a(\lambda_x, w) \;\; \text{for all } w \in V^{\mathrm{f}}_h(\omega_{x,k})$$

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 $u_{H,k}^{\mathrm{ms},h} \in V_{H,k}^{\mathrm{ms},h}$ satisfies

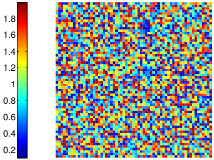
$$a(u_{H,k}^{\mathrm{ms},h}, v) = F(v) \quad \text{for all } v \in V_{H,k}^{\mathrm{ms},h}$$

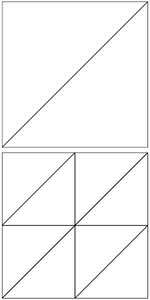
Theorem (Error estimate)

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

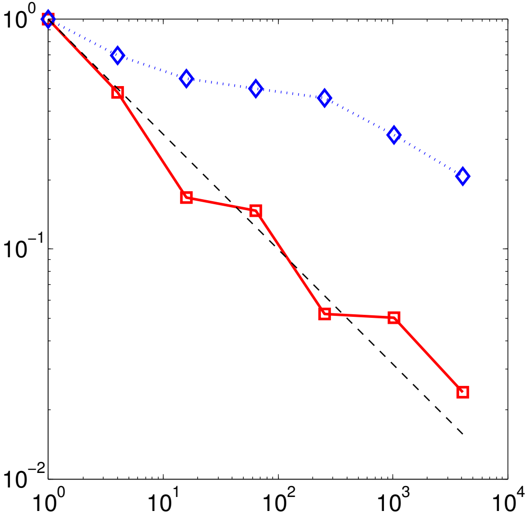
holds with a constant C_3 that does not depend on H, h, f, or u.

Numerical experiment I



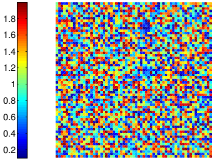


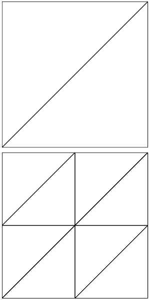
$H = 2^{-1}, 2^{-2}, \ldots, 2^{-7}$
$h = 2^{-9}$, $k = \log(1/H)$



$|||u_h - u_{H,k}^{\mathrm{ms},h}|||$ vs. #dof

Numerical experiment I





$$H = 2^{-1}, 2^{-2}, \ldots, 2^{-7}$$
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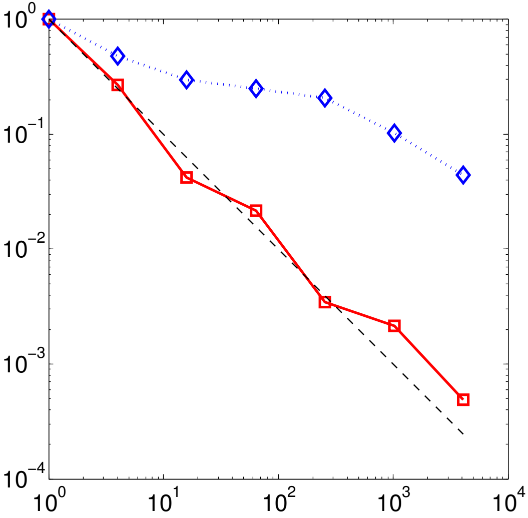
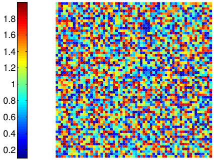
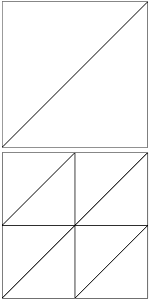


$\|u_h - u_{H,k}^{\text{ms},h}\|$ vs. #dof

Numerical experiment I





$H = 2^{-1}, 2^{-2}, \dots, 2^{-7}$
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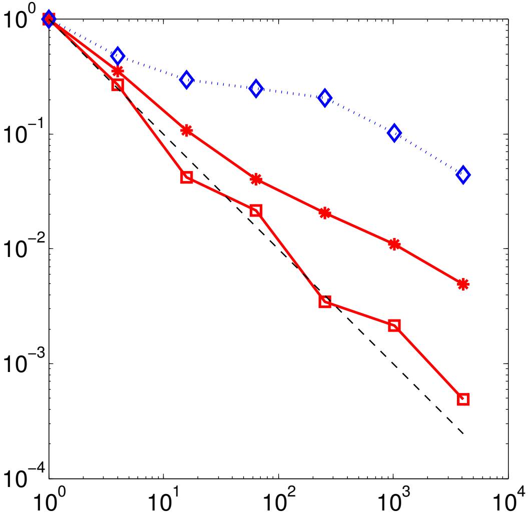
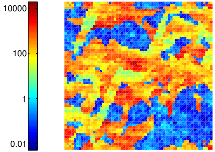
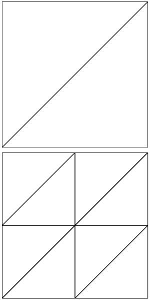


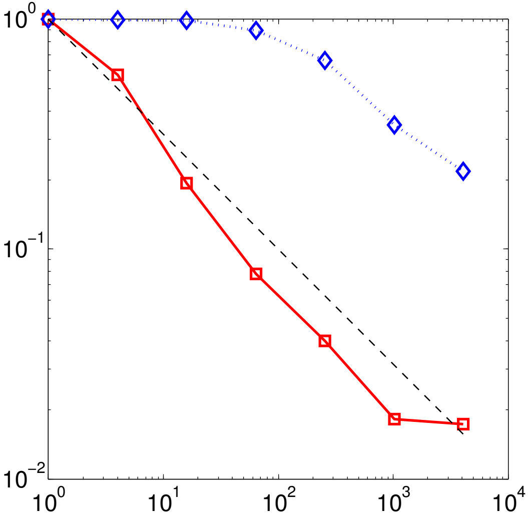
$\|u_h - \mathfrak{I}_\mathcal{T} u^{\mathrm{ms},h}_{H,k}\|$ vs. #dof

Numerical experiment II



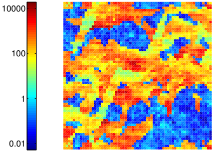


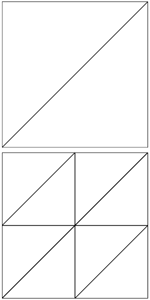
$H = 2^{-1}, 2^{-2}, \ldots, 2^{-7}$
$h = 2^{-9}$, $k = \log(1/H)$



$|||u_h - u_{H,k}^{\mathrm{ms},h}|||$ vs. #dof

Numerical experiment II





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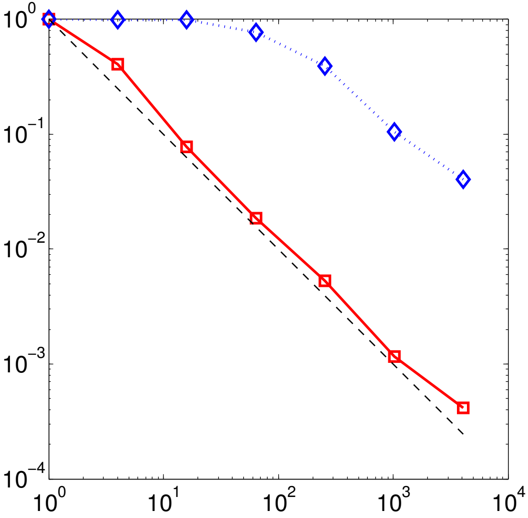
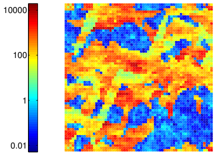
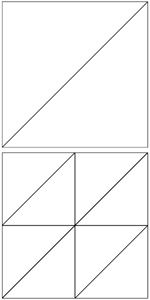
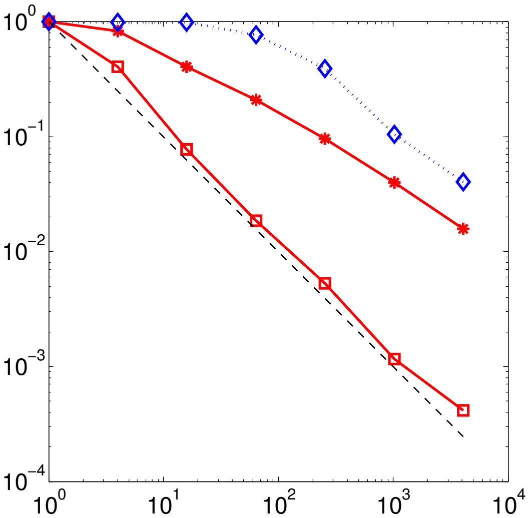


$\|u_h - u_{H,k}^{ms,h}\|$ vs. #dof

Numerical experiment II







$H = 2^{-1}, 2^{-2}, \ldots, 2^{-7}$
$h = 2^{-9}$, $k = \log(1/H)$

$\|u_h - \mathfrak{I}_{\mathcal{T}} u^{\mathrm{ms},h}_{H,k}\|$ vs. #dof

Outline

Semi-linear PDE's

We consider with F monotone and Lipschitz continuous,

$$-\nabla \cdot A\nabla u + F(u, \nabla u) = g, \text{ in } \Omega \quad u = 0 \text{ on } \partial\Omega,$$

and let $u_H^{\mathrm{ms}} \in \operatorname{span}\{\lambda_x - \phi_x \mid x \in \mathcal{N}\}$ be the multiscale approximation.

Lemma

$$\|\nabla(u - u_H^{\mathrm{ms}})\|_{L^2(\Omega)} \lesssim \gamma^k \|f\|_{L^2(\Omega)} + \|Hf\|_{L^2(\Omega)}.$$

- Same basis as in linear case is used i.e. same decay rate.
- The basis will not change in the non-linear iteration.

P. Henning, A. Målqvist, and D. Peterseim.
A localized orthogonal decomposition method for semi-linear elliptic problems.
Mathematical Modelling and Numerical Analysis, 2014.

Eigenvalue Problems

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

$$-\nabla \cdot A\nabla u = \lambda u, \text{ in } \Omega \quad u = 0 \text{ on } \partial\Omega.$$

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

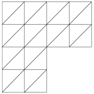
$$a(u_H^{\mathrm{ms}}, v) = \lambda_H(u_H^{\mathrm{ms}}, v), \quad \forall v \in V_H^{\mathrm{ms}}.$$

Theorem

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

A. Målqvist and D. Peterseim.
Computation of eigenvalues by numerical upscaling. *in review Numerische Mathematik*.

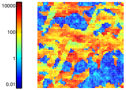
Eigenvalue Problem

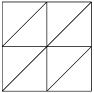


ℓ	$\lambda_h^{(\ell)}$	$e^{(\ell)}(1/2\sqrt{2})$	$e^{(\ell)}(1/4\sqrt{2})$	$e^{(\ell)}(1/8\sqrt{2})$	$e^{(\ell)}(1/16\sqrt{2})$
1	9.6436869	0.003494567	0.000034466	0.000000546	0.000000010
2	15.1989274	0.009621397	0.000079887	0.000000845	0.000000010
3	19.7421815	0.023813222	0.000213097	0.000002073	0.000000023
4	29.5281571	0.096910157	0.000724615	0.000006574	0.000000076
5	31.9265496	0.094454625	0.000874659	0.000009627	0.000000138
6	41.4922250	-	0.002395227	0.000019934	0.000000254
7	44.9604884	-	0.002443271	0.000019683	0.000000223
8	49.3631826	-	0.003651870	0.000028869	0.000000308
9	49.3655623	-	0.004266472	0.000032835	0.000000355
10	56.7389993	-	0.006863742	0.000055219	0.000000618
11	65.4085991	-	0.011534878	0.000082414	0.000000856
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 $h = 2^{-7}\sqrt{2}$.

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	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 $h = 2^{-7}\sqrt{2}$.

Outline

Current and future work

- Gross-Pitaevskii equation,

$$-\Delta u + Vu + u^3 = \lambda u, \quad \|u\|_{L^2(\Omega)} = 1.$$

- Time dependent problems, parabolic and hyperbolic.
- Quadratic eigenvalue problems: damped systems,

$$Kx + \lambda Cx + \lambda^2 Mx = 0.$$

- Nonlinear systems modeling two phase flow (in collaboration with geoscience in Uppsala).
- Applications in material science.
- Main mathematical challenge: Convergence independent of aspect ratio.