On convergence of multiscale methods

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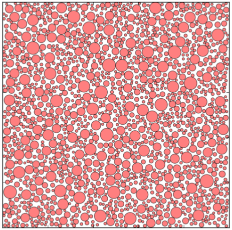
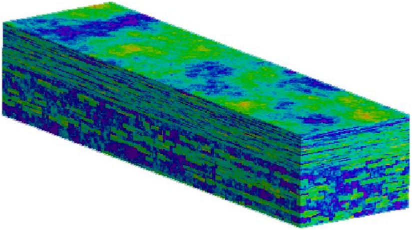
Multiscale problems

Applications such as



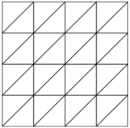


▷ composite materials ▷ flow in a porous medium

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

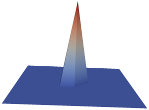
Major challenge: Features on multiple non-separated scales.

Finite elements (FE) – methodology



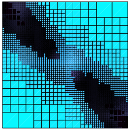
The numerical solution of PDEs by FEM consists of

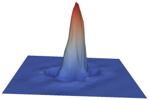
- construction of an "appropriate" FE mesh
- choosing (local) basis functions (of variable degree of approximation)



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





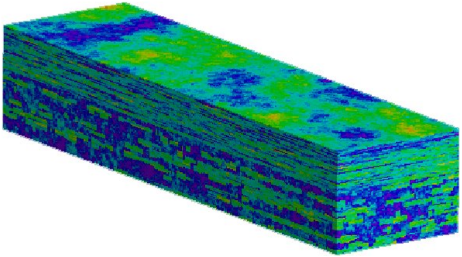
Outline

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 $0 < \alpha \leq A \in L^\infty(\Omega)$



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

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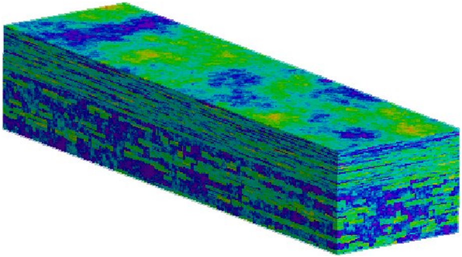

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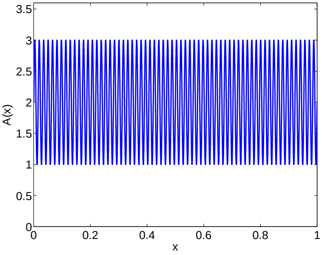
Example (periodic coefficient): $A(x) = 2 + \sin(2\pi x/\varepsilon)$, $\varepsilon = 2^{-6}$, $f = 1$



oscillatory coefficient

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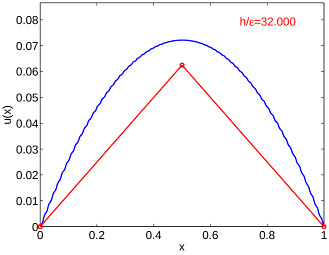
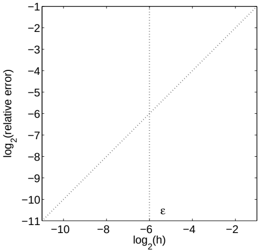


solution and P1-FEM-approximation



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

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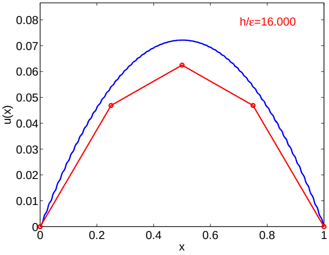

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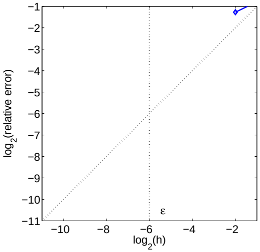

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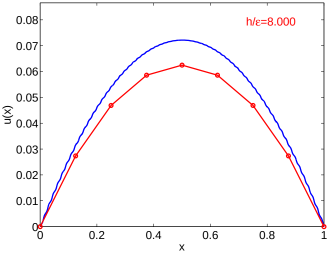

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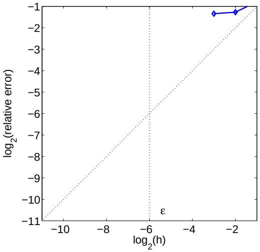

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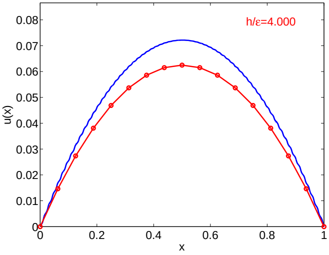

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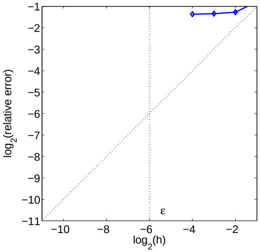

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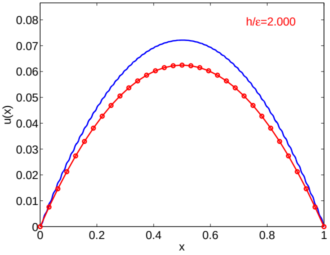

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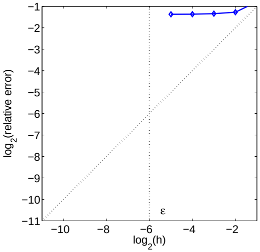

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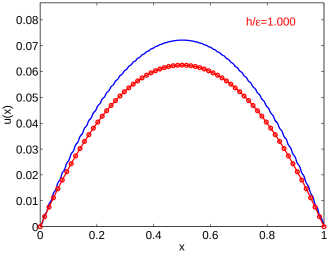

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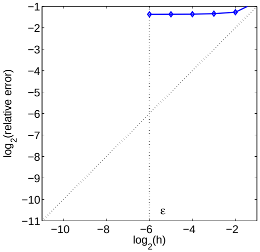

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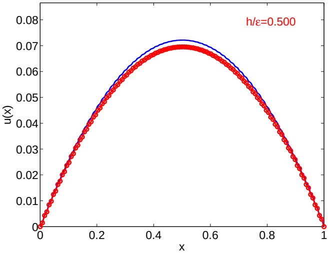

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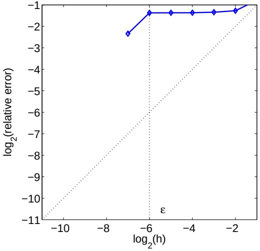

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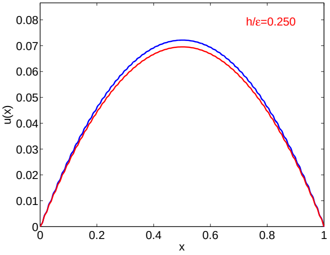

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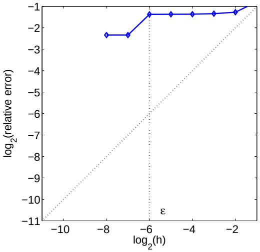

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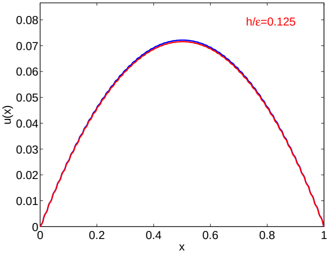

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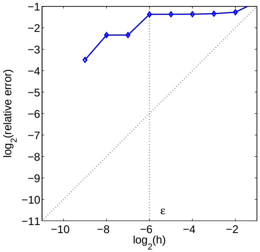

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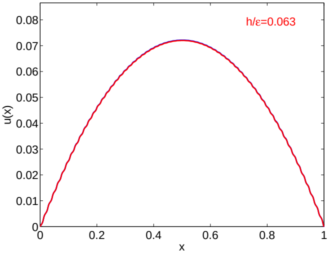

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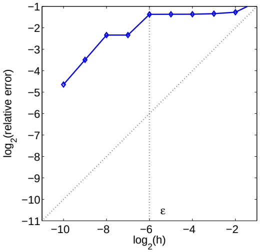

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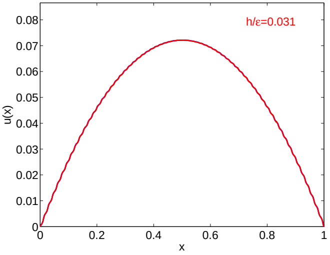

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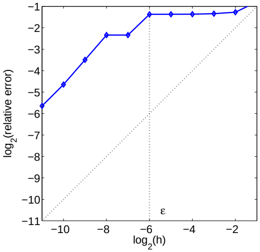

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Examples (periodic coefficients)

- 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.
- This implies that huge linear systems need to be solved in each time step in the oil reservoir application. Furthermore, the stiffness matrices changes in each time step.

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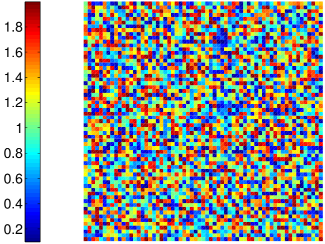
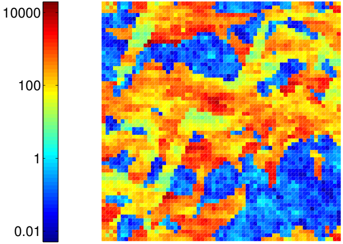
Examples (rough coefficients)



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 diameter $\approx \log(1/H)$
- 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.
ArXiv e-prints, Oct. 2011.

Some known methods

- Upscaling techniques: Durlofsky et al. 98, Nielsen et al. 98
- Variational multiscale method: Hughes et al. 95, Arbogast 04, Larson-Målqvist 05, Nolen et al. 08, Nordbotten 09
- 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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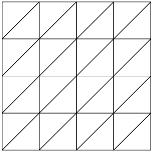
Remark

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

Outline

Multiscale decomposition

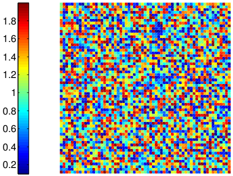
- (coarse) FE mesh $\mathcal{T}$ with parameter H
- P1-FE space $V_H := \{v \in V \mid \forall T \in \mathcal{T}, v|_T \in P_1(T)\}$
- $\mathfrak{I}_{\mathcal{T}} : V \to V_H$ quasi-interpolation operator



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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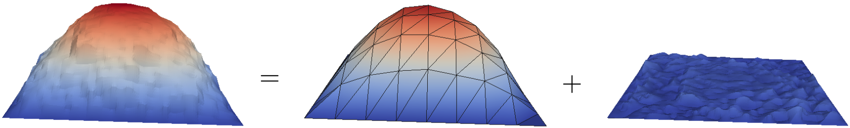


$u \in V$ = $u_H \in V_H$ + $u^{\mathrm{f}} \in V^{\mathrm{f}}$

Orthogonalization

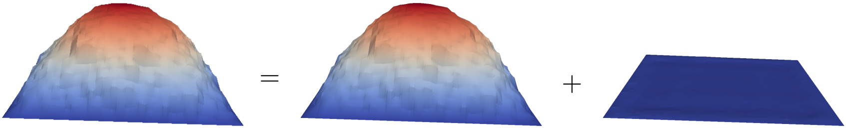
- For each $v \in V_H$ define finescale projection $\mathfrak{F}v \in V^{\mathrm{f}}$ by

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

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:



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

Error analysis (perfect decomposition)

Lemma

$$|||u - u_H^{\mathrm{ms}}||| \leq C_{\mathrm{ol}} C_{\mathfrak{I}_\mathcal{T}} \alpha^{-1} \|Hf\|_{L^2(\Omega)}$$

Sketch of proof:

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

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

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

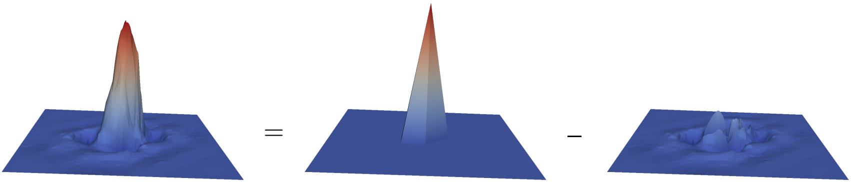
Modified nodal basis

- $\mathcal{N}$ 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

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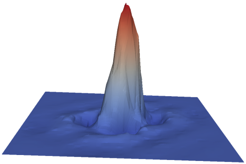
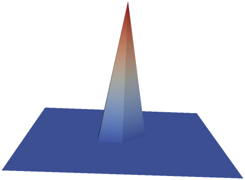


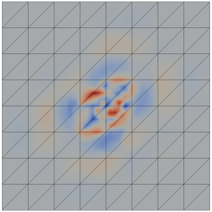
$\lambda_x - \phi_x \in V_H^{\mathrm{ms}}$

$=$



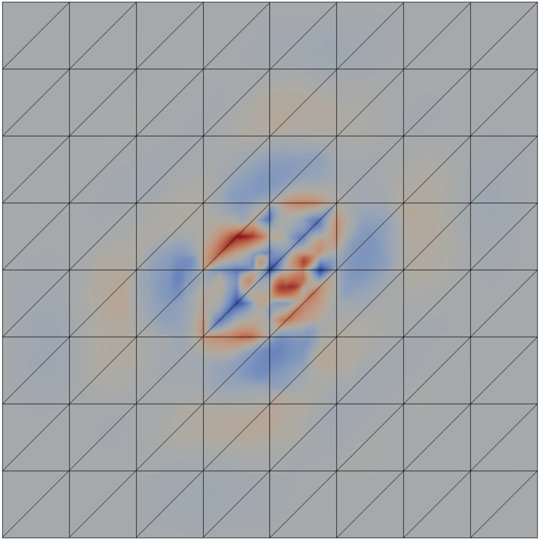
$\lambda_x \in V_H$

$-$



$\phi_x \in V^{\mathrm{f}}$

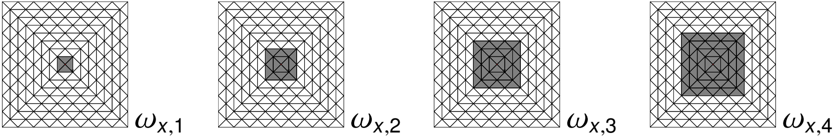
Modified nodal basis



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

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

The multiscale method

Multiscale approximation seeks $u_{H,k}^{\text{ms}} \in V_{H,k}^{\text{ms}}$ such that

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

Remarks:

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

Error Analysis

Lemma (Truncation error)

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

$$|||\phi_x - \phi_{x,\ell k}|||^2 \leq C_1 \gamma^k |||\phi_x|||^2.$$

Sketch of proof:

- By introducing a cut of function $\zeta_{x,\ell k} = 0$ in $\omega_{x,\ell(k-1)}$ and $\zeta_{x,\ell k} = 1$ in $\Omega \setminus \omega_{x,\ell k}$ we conclude: ($(1-\zeta_{x,\ell k})\phi_x \in V^{\mathrm{f}}(\omega_{\ell k})$) $|||\phi_x - \phi_{x,\ell k}||| \lesssim |||\zeta_{x,\ell k}\phi_x||| \lesssim \|\zeta_{x,\ell k}\|_{L^\infty(\Omega)} |||\phi_x|||_{\Omega\setminus\omega_{x,\ell(k-1)}} + \|\nabla\zeta_{x,\ell k}\|_{L^\infty(\Omega)} \|\phi_x - \mathfrak{I}_{\mathcal{T}}\phi_x\|_{L^2(\Omega\setminus\omega_{x,\ell(k-1)})} \lesssim |||\phi_x|||_{\Omega\setminus\omega_{x,\ell(k-1)}}$.
- $|||\phi_x|||^2_{\Omega\setminus\omega_{x,\ell(k-1)}} \leq (A\zeta^2_{x,\ell(k-1)}\nabla\phi_x, \nabla\phi_x) = (A\nabla\phi_x, \nabla(\zeta^2_{x,\ell(k-1)}\phi_x)) - 2(A\zeta_{x,\ell(k-1)}\phi_x\nabla\zeta_{x,\ell(k-1)}, \nabla\phi_x) \lesssim \ell^{-1}\|H^{-1}\|_{L^\infty(\Omega)}\|\phi_x\|_{L^2(\Omega\setminus\omega_{x,\ell(k-2)})}|||\phi_x|||_{\Omega\setminus\omega_{x,\ell(k-2)}} \lesssim \ell^{-1}|||\phi_x|||^2_{\Omega\setminus\omega_{x,\ell(k-2)}}$.
- Repeat $|||\phi_x|||^2_{\Omega\setminus\omega_{x,\ell(k-1)}} \lesssim (C_2/\ell)^{k-1}|||\phi_x|||^2 := \gamma^k|||\phi_x|||^2$.

Error Analysis

Theorem (Main result)

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

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

Sketch of proof:

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

Error Analysis

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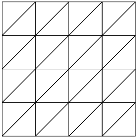
Theorem holds without any assumptions on scales or regularity!

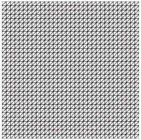
Outline

Full discretization

- Finescale mesh



$\mathcal{T}$ mesh refinement $\rightsquigarrow$



$\mathcal{T}_h$ 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

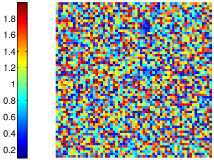
$$a(u_{H,k}^{\mathrm{ms},h}, v) = F(v) \quad \text{for all } v \in V_{H,k}^{\mathrm{ms},h}$$

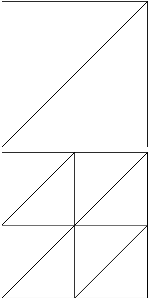
Theorem (Error estimate)

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

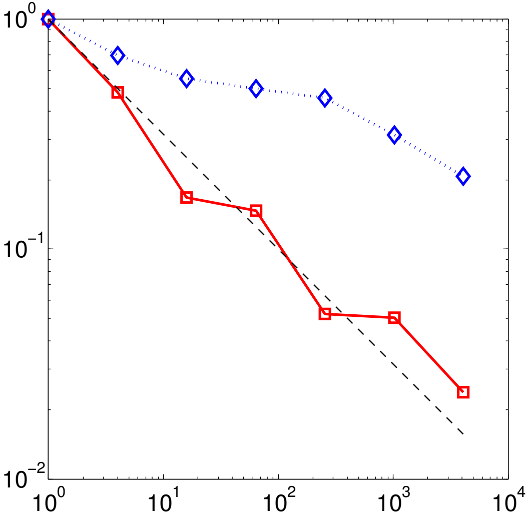
holds with a constant C_3 that does not depend on H, h, k, f, or u.

Numerical experiment I



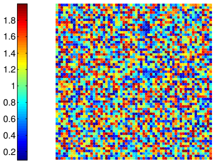


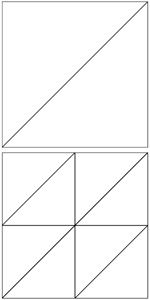
$$H = 2^{-1}, 2^{-2}, \ldots, 2^{-7}$$
$$h = 2^{-9},\ k = \log(1/H)$$



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

Numerical experiment I





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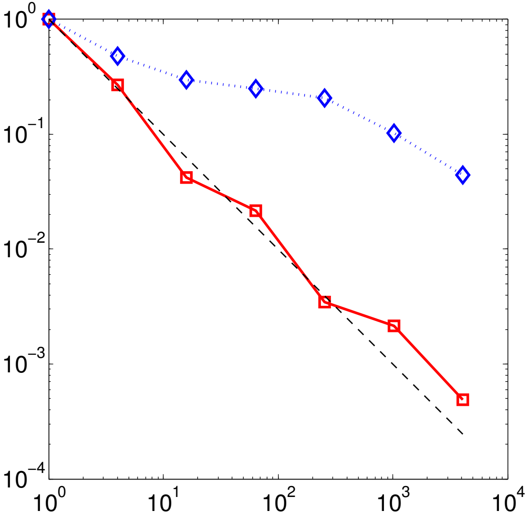
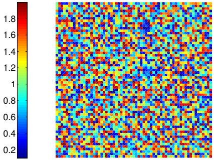
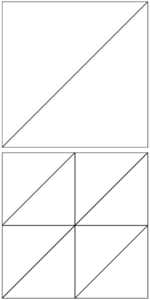


$\|u_h - u_{H,k}^{\mathrm{ms},h}\|$ vs. #dof

Numerical experiment I





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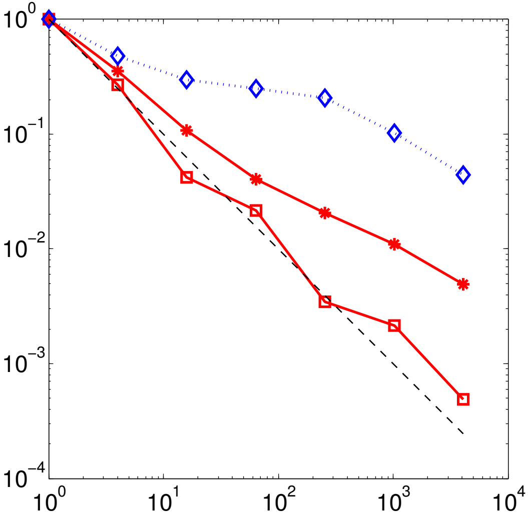
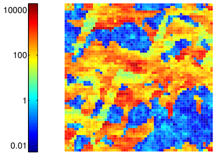
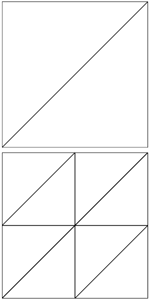
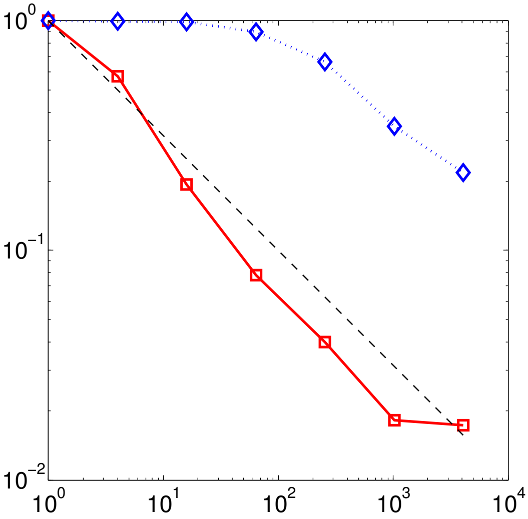


$\|u_h - \mathfrak{I}_\mathcal{T} u_{H,k}^{\mathrm{ms},h}\|$ vs. #dof

Numerical experiment II







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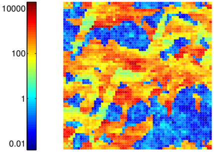
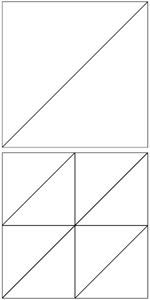
$|||u_h - u_{H,k}^{\mathrm{ms},h}|||$ vs. #dof

Numerical experiment II





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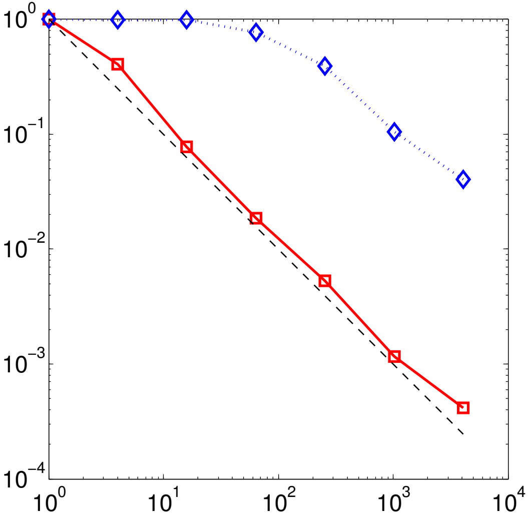
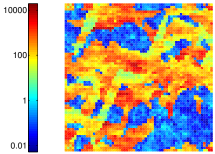
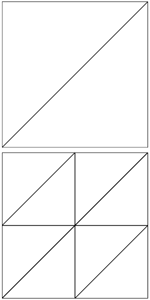


$\|u_h - u_{H,k}^{ms,h}\|$ vs. #dof

Numerical experiment II





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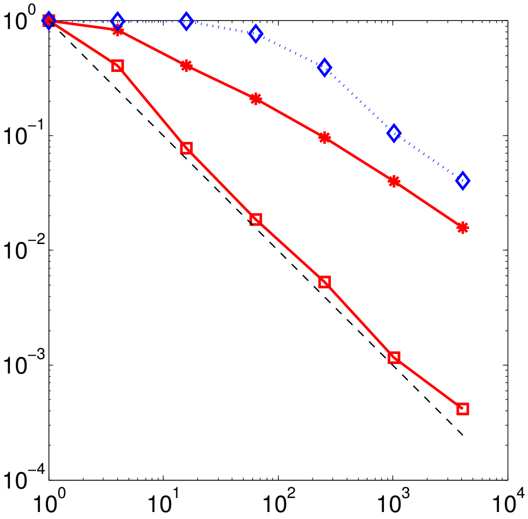


$\|u_h - \mathfrak{I}_\mathcal{T} u^{\mathrm{ms},h}_{H,k}\|$ vs. #dof

Outline

Ongoing work

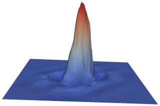
The key is to simplify the computation of the modified basis and to reuse the multiscale basis in the computation.

- Advection-diffusion-reaction equations.
- Semi-linear partial differential equations.
- Time dependent problems.

We will use the same construction as above for all these applications, namely: Find $\phi_x \in V^{\mathrm{f}}$ such that

$$(A\nabla\phi_x, \nabla w) = (A\nabla\lambda_x, \nabla w), \quad \text{for all } w \in V^{\mathrm{f}},$$

$V_H^{\mathrm{ms}} = \operatorname{span}(\{\lambda_x - \phi_x\})$, and $x \in \mathcal{N}$.



Advection-diffusion-reaction equations

Let $u \in V$ solve,

$$-\nabla \cdot A\nabla u + B\nabla u + Cu = f, \text{ in } \Omega \quad u = 0 \text{ on } \partial\Omega,$$

where $A, B, C \in L^\infty(\Omega)$ such that the problem is well posed.

It holds,

$$\|A^{1/2}\nabla(u - u_H^{\mathrm{ms}})\|_{L^2(\Omega)}^2 \lesssim$$

$$\alpha^{-1/2}\|H^{1+s}D^s f\|_{L^2(\Omega)} + \alpha^{-1}H\Big(\|B\|_{L^\infty(\Omega)} + H\|C - \nabla \cdot B\|_{L^\infty(\Omega)}\Big)\|g\|_{H^{-1}(\Omega)},$$

with $s \leq 2$, for underlying finite elements of degree 1.

- Note that even for large advection and reaction terms we get good approximation, even though only A is considered in the construction of the basis.

Semi-linear PDE's

Let $u \in V$ solve,

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

where F is monotone and Lipschitz cont. in both arguments (L_F).

It holds,

$$\|A^{1/2}\nabla(u - u_H^{\text{ms}})\|_{L^2(\Omega)} \lesssim \alpha^{-1/2}\|H(f - \mathfrak{I}_{\mathcal{T}} f)\|_{L^2(\Omega)} + \alpha^{-1} H L_F \|f\|_{H^{-1}(\Omega)}$$

without using information from F in the construction of the coarse multiscale space V_H^{ms}.

- For lowest order nonlinearity $F(u, \nabla u) = C(u)$ we even get $\alpha^{-1/2}\|H(f - \mathfrak{I}_{\mathcal{T}} f)\|_{L^2(\Omega)} + \alpha^{-1} H^2 L_F \|f\|_{H^{-1}(\Omega)}$
- This means that the coarse basis can be used without modification throughout the full non-linear iteration.

Time dependent problems

Let $u \in V$ solve,

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

with initial value $u(0) = 0$. For A independent of time we get,

$$\tfrac{1}{2}\|u(T) - u_H^{\mathrm{ms}}(T)\|_\Omega^2 + \int_0^T \|A^{1/2}\nabla(u - u_H^{\mathrm{ms}})\|_{L^2(\Omega)}^2 \, dt \lesssim \alpha^{-2} \int_0^T \|H(f - \Im_{\mathcal{T}} f)\|_{L^2(\Omega)}^2 \, dt.$$

- The approximation is only discretized in space.
- With $A = A(t)$ one can discretize in time, and in each time step modify the basis if $A(t_{n+1}) - A(t_n)$ is large enough.

Oil reservoir simulation

Find pressure p and water concentration s such that:

$$-\nabla \cdot k\mu(s)\nabla p = q, \quad \dot{s} - \nabla \cdot [f(s)\mu(s)k\nabla p] = g.$$

A combination of these results will provide good insight into how to construct a multiscale method for the entire system.

Outline

Conclusion

- A new variational multiscale FEM yields scale-independent textbook convergence and, hence, establishes reliable computational approximation of multiscale problems.
- Numerical experiments confirms the theoretical results. Furthermore numerical results are not sensitive to high contrast.
- Numerical examples confirms rapid decrease in error for very challenging permeability coefficients.
- Multiscale basis functions are very useful for many interesting applications such as, convection-diffusion-reaction problems, semi linear problems, and parabolic problems.

Outlook

- Treatment of high contrast also in the analysis, error bound for $\mathfrak{I}_{\mathcal{T}} u_{H,k}^{\mathrm{ms},h}$, and error bounds in $L^2(\Omega)$ norm.
- Design and analysis of reliable multiscale methods hyperbolic problems.
- Design of a multiscale approach to the full two phase flow system.
- Consider uncertainty in the coefficient and construct efficient algorithms for computing statistical information, such as distribution function, of output quantities of interest.
- Daniel will talk about adaptivity on the 8th of October.