

On convergence of multiscale methods

Axel Målqvist Daniel Peterseim

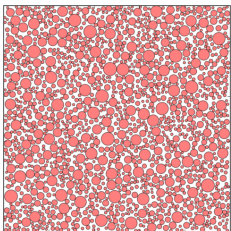
Uppsala University

Humboldt Universität

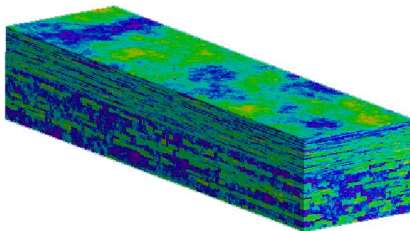
2012-09-20

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**.

Multiscale problems

Example: Oil reservoir simulation



Find pressure p and water concentration s such that:

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

where $\mathbf{k}$ is permeability, $\mu(s)$ the total mobility, f fractional flow, and g, q sink and source terms.

Multiscale problems

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Find pressure p and water concentration s such that:

$$-\nabla \cdot \mathbf{k} \mu(s_n) \nabla p_{n+1} = q, \quad \frac{s_{n+1} - s_n}{\Delta t} - \nabla \cdot [f(s_n) \mu(s_n) \mathbf{k} \nabla p_{n+1}] = g,$$

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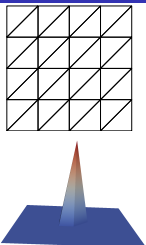
$$-\nabla \cdot k \mu(s_n) \nabla p_{n+1} = q, \quad \frac{s_{n+1} - s_n}{\Delta t} - \nabla \cdot [f(s_n) \mu(s_n) k \nabla p_{n+1}] = g,$$

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Finite elements (FE) – methodology

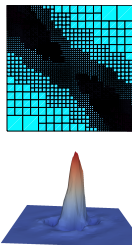
The numerical solution of PDEs by FEM consists of

- 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



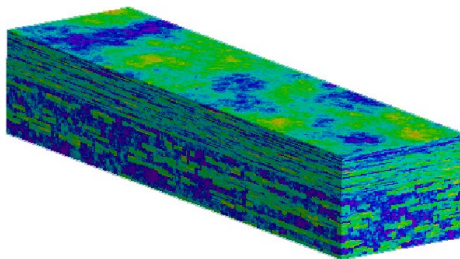
- 1 **Setting and Motivation**
- 2 Multiscale Method and Convergence
- 3 Full Discretization and Numerical Experiments
- 4 Adaptivity
- 5 Ongoing Work
- 6 Conclusion

Model multiscale problem

Poisson's equation

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

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

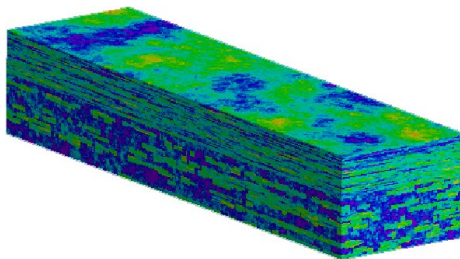


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Poisson's equation (variational form): $u \in V := H_0^1(\Omega)$ s.t.

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

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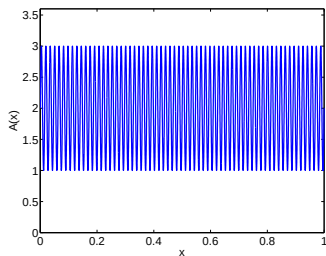
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Example (periodic coefficient): $A(x) = 2 + \sin(2\pi x/\varepsilon)$, $\varepsilon = 2^{-6}$, $f = 1$



oscillatory coefficient

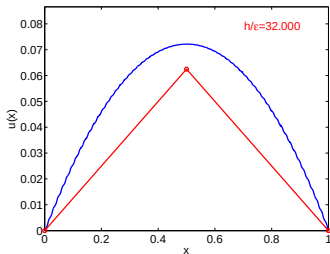
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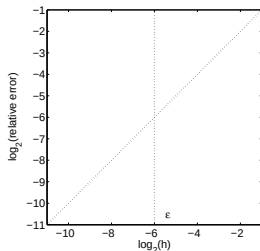
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solution and P1-FEM-approximation



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

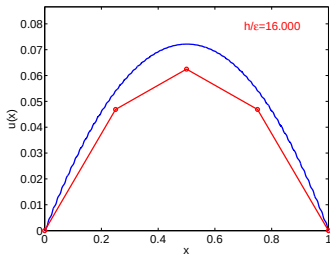
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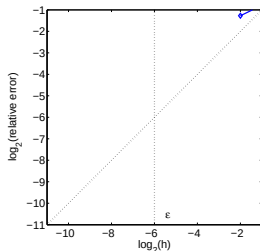
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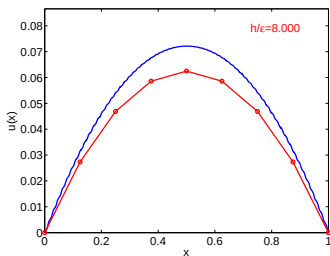
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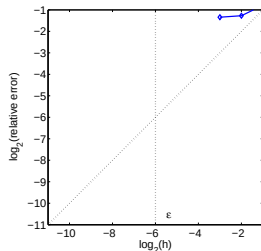
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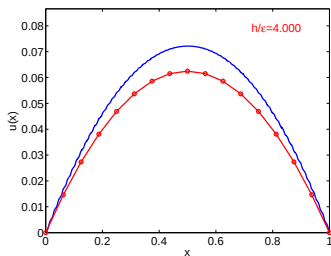
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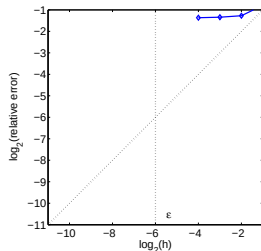
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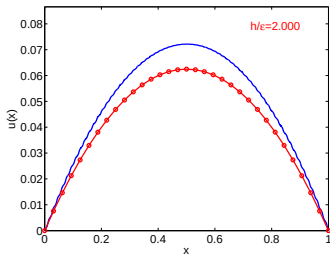
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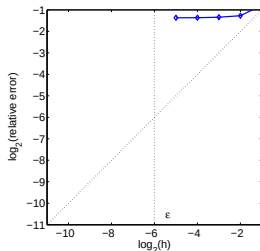
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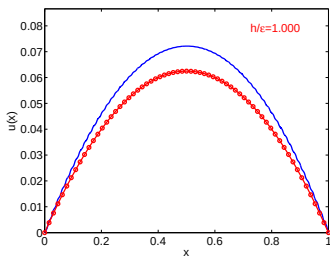
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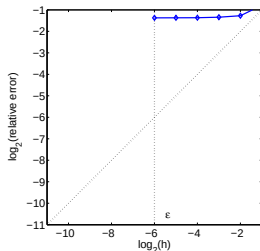
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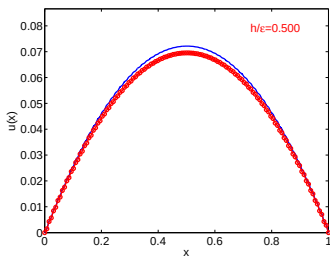
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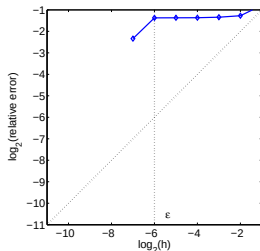
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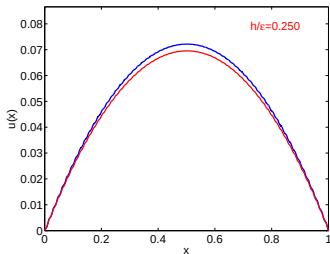
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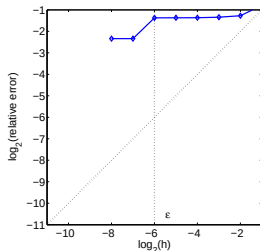
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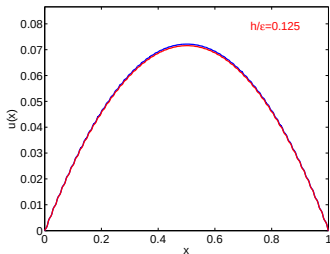
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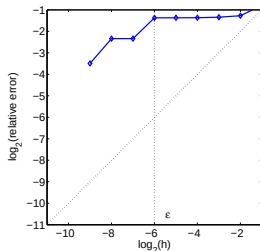
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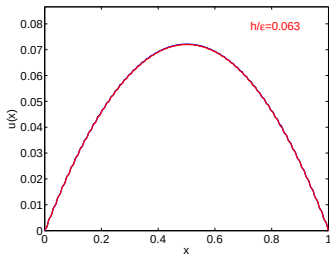
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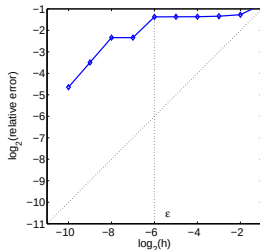
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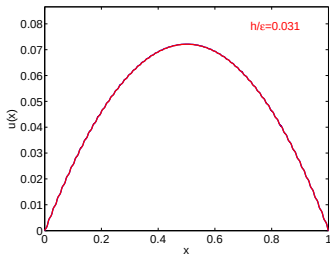
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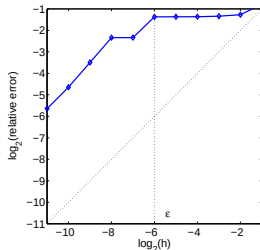
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Examples (periodic coefficients)

- We have $\|u - u_h\| := \|\mathbf{A}^{1/2} \nabla(u - u_h)\| \leq C(A, f)h = C'(f)\frac{h}{\epsilon}$.
- 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.

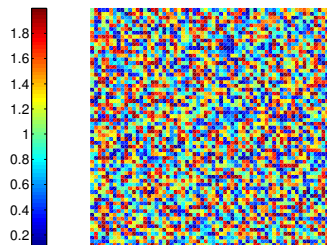
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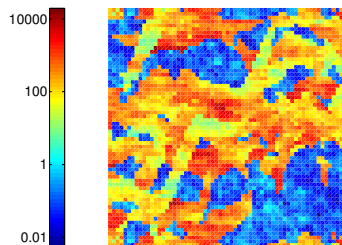
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Examples (rough coefficients)



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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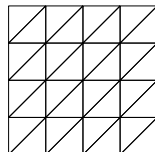
Remark

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

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Multiscale decomposition

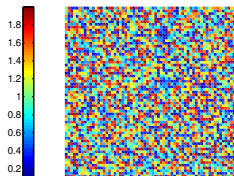
- (coarse) FE mesh $\mathcal{T}$ with parameter H
- P1-FE space $V_H := \{v \in V \mid \forall T \in \mathcal{T}, v|_T \in P_1(T)\}$
- $\mathfrak{I}_{\mathcal{T}} : V \rightarrow V_H$ quasi-interpolation operator



Decomposition

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

Example:



rough coefficient

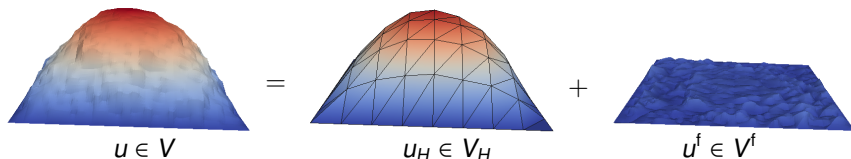
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Orthogonalization

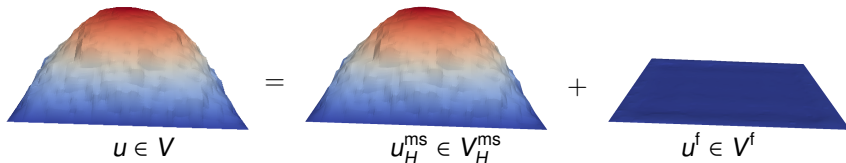
- For each $v \in V_H$ define finescale projection $\mathfrak{F}v \in V^f$ by

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

Orthogonal Decomposition

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

Example:



Error analysis (perfect decomposition)

Lemma

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

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 $u^{\text{f}} := u - u_H^{\text{ms}} \in V^{\text{f}}$
- $\mathfrak{I}_{\mathcal{T}} u^{\text{f}} = 0$, interpolation error estimate, and finite overlap of the patches ω_T conclude the proof

$$\begin{aligned} |||u^{\text{f}}|||^2 &= a(\underbrace{u^{\text{f}} + u_H^{\text{ms}}}_{=u}, u^{\text{f}}) = F(u^{\text{f}}) = F(u^{\text{f}} - \mathfrak{I}_{\mathcal{T}} u^{\text{f}}) \\ &\leq \sum_{T \in \mathcal{T}} \|f\|_{L^2(T)} \|u^{\text{f}} - \mathfrak{I}_{\mathcal{T}} u^{\text{f}}\|_{L^2(T)} \leq C_{\text{ol}} C_{\mathfrak{I}_{\mathcal{T}}} \alpha^{-1} \|Hf\|_{L^2(\Omega)} |||u^{\text{f}}||| \quad \square \end{aligned}$$

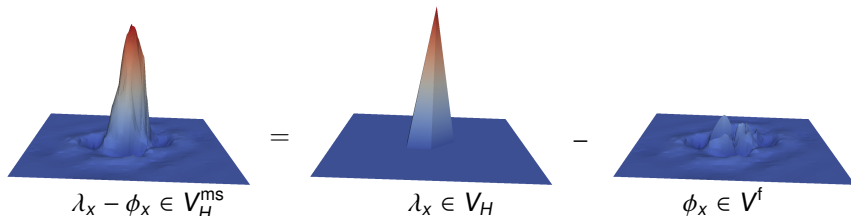
Modified nodal basis

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

Ideal multiscale FE space

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

Example



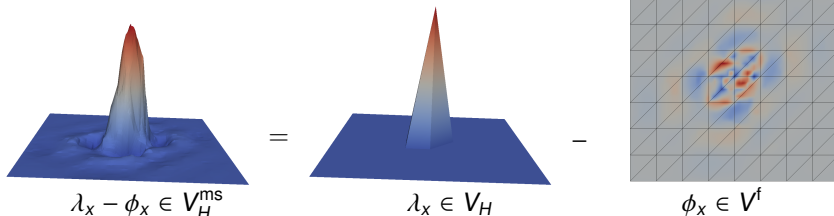
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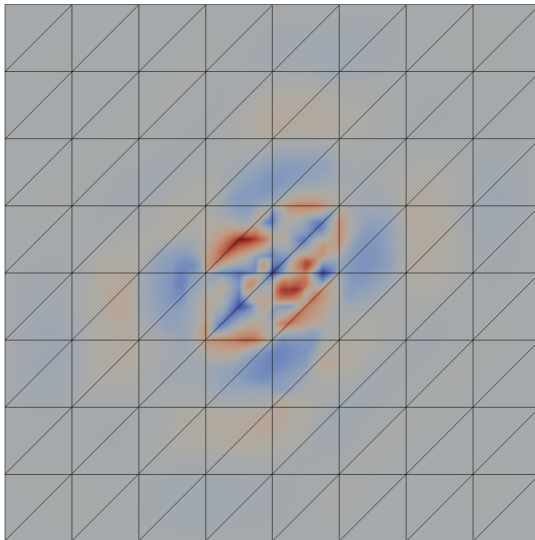
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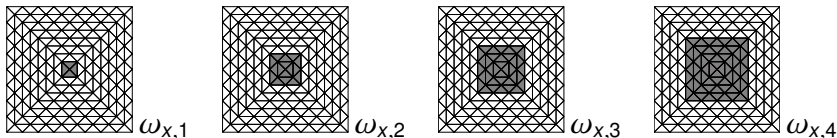
Modified nodal basis



Assuming more regularity on A we have $\lambda_x - \phi_x \in H^2(\Omega) \cap H_0^1(\Omega)$.

Localization

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



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

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

Localized multiscale FE spaces

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

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

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

Theorem (Main result)

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

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

Error analysis

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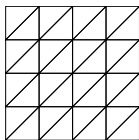
holds with a constant C_2 that does not depend on H , k , f , or u .

Theorem holds without any assumptions on scales or regularity!

- 1 Setting and Motivation
- 2 Multiscale Method and Convergence
- 3 **Full Discretization and Numerical Experiments**
- 4 Adaptivity
- 5 Ongoing Work
- 6 Conclusion

Full discretization

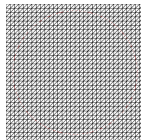
- Finescale mesh



$\mathcal{T}$

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 $\phi_{x,k}^h \in V_h^f(\omega_{x,k}) := V^f(\omega_{x,k}) \cap V_h$ satisfy

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

Full discretization

Fully discrete multiscale FE spaces

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

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

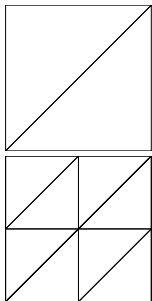
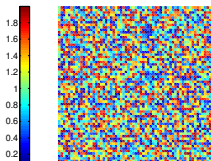
$$a(u_{H,k}^{\text{ms},h}, v) = F(v) \quad \text{for all } v \in V_{H,k}^{\text{ms},h}$$

Theorem (Error estimate)

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

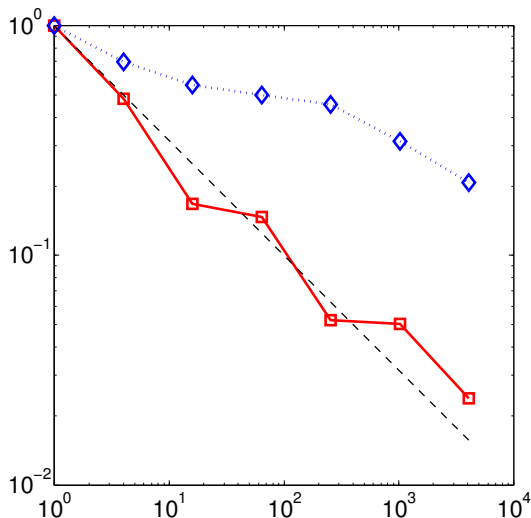
holds with a constant C_3 that does not depend on H , h , k , f , or u .

Numerical experiment I



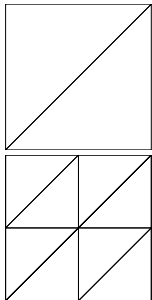
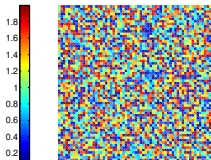
$$H = 2^{-1}, 2^{-2}, \dots, 2^{-7}$$

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



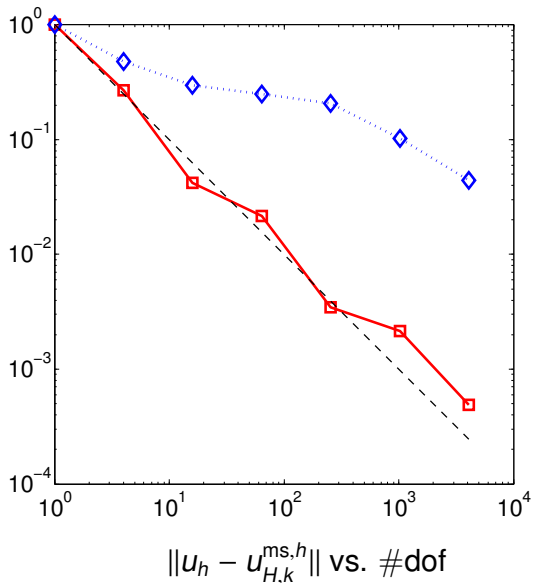
$|||u_h - u_{H,k}^{ms,h}|||$ vs. #dof

Numerical experiment I

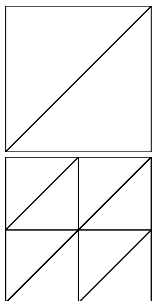
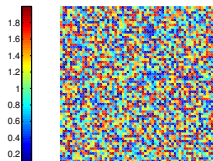


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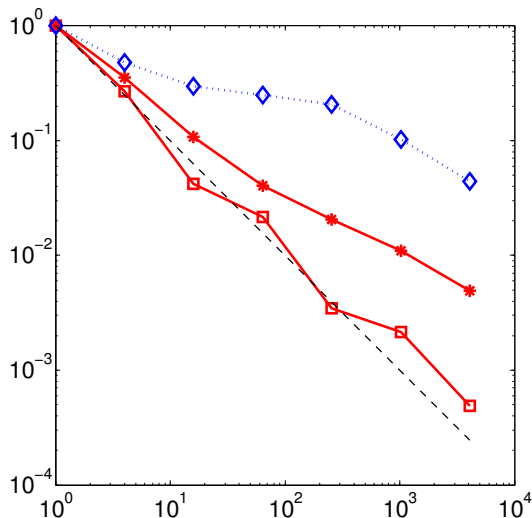


Numerical experiment I



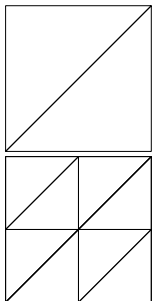
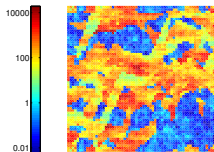
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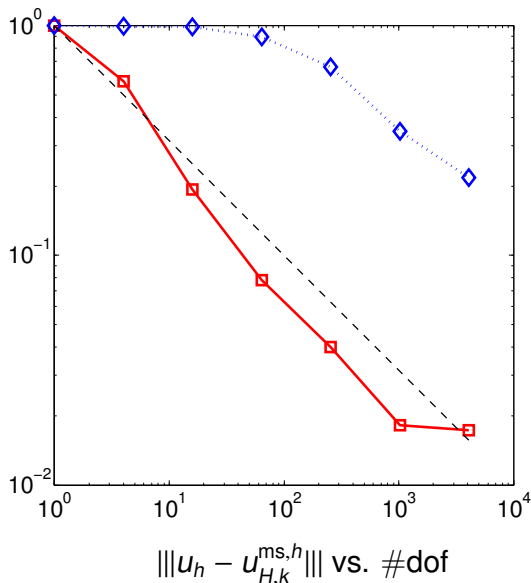
$\|u_h - \mathfrak{I}_{\mathcal{T}} u_{H,k}^{ms,h}\|$ vs. #dof

Numerical experiment II

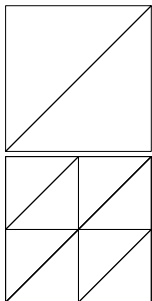
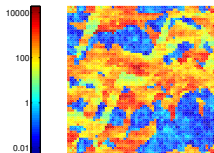


$$H = 2^{-1}, 2^{-2}, \dots, 2^{-7}$$

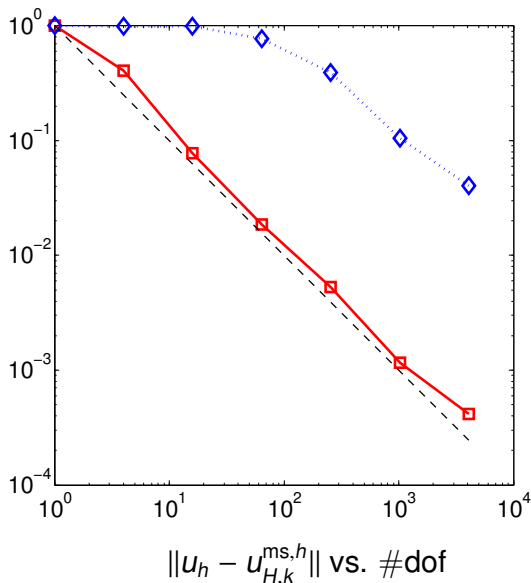
$$h = 2^{-9}, k = \log(1/H)$$



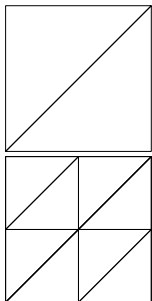
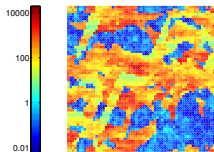
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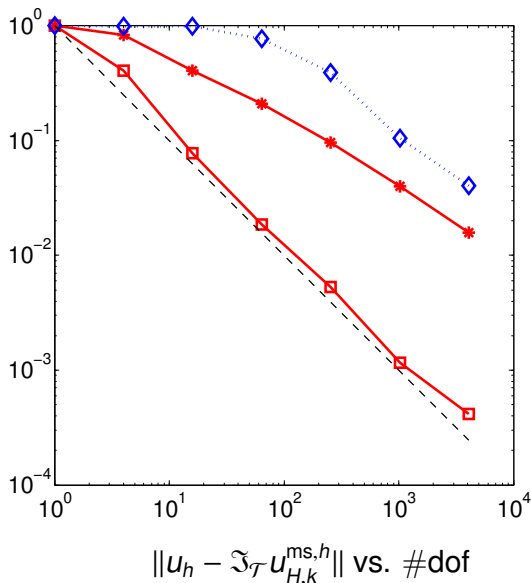


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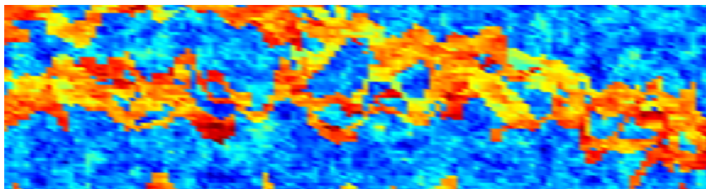


- 1 Setting and Motivation
- 2 Multiscale Method and Convergence
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- 4 **Adaptivity**
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- 6 Conclusion

A posteriori error estimation and adaptivity

Motivation:

- The method we propose will have overlapping patches, which (especially in 3D) is expensive.
- The problems we consider often includes channels so the solution is typically somewhat localized in space.
- The size of the patches and the refinement level is difficult to predict a priori, we therefore need error indicators to tune these parameters automatically.



A posteriori error estimation and adaptivity

Let $\rho^2(v) = \sum_{K \in \mathcal{T}_h} h_K^2 \|\nabla \cdot A \nabla v\|_{L^2(K)}^2 + h_K \| [n \cdot A \nabla v] \|_{L^2(\partial K)}^2$.

Theorem

$$\begin{aligned} \|u - u_{H,k}^{\text{ms},h}\|^2 &\leq C \|Hf\|_{L^2(\Omega)}^2 + C(u_{H,k}^{\text{ms},h}) \sum_{x \in \mathcal{N}} \rho^2(\lambda_x - \phi_{x,k}^h) \\ &\quad + C(u_{H,k}^{\text{ms},h}) \sum_{x \in \mathcal{N}} H \|n \cdot A \nabla \phi_{x,k}^h\|_{L^2(\partial \omega_{x,k})}^2 \end{aligned}$$

- Effect of coarse mesh size included in first term.
- A standard element indicator on each patch measuring the effect of decreasing fine scale mesh size h .
- A new indicator on the boundary of each patch $\partial \omega_{x,k}$. The a priori analysis shows that $\phi_{x,k}^h$ decays exponentially in k .

A posteriori error estimation and adaptivity

Let $\rho^2(v) = \sum_{K \in \mathcal{T}_h} h_K^2 \|\nabla \cdot A \nabla v\|_{L^2(K)}^2 + h_K \|[n \cdot A \nabla v]\|_{L^2(\partial K)}^2$.

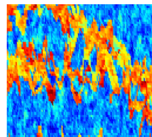
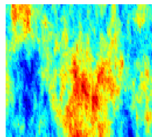
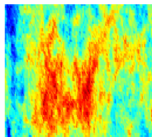
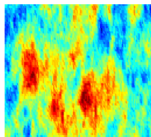
Theorem

$$\begin{aligned} \|u - u_{H,k}^{\text{ms},h}\|^2 &\leq C \|Hf\|_{L^2(\Omega)}^2 + C(u_{H,k}^{\text{ms},h}) \sum_{x \in \mathcal{N}} \rho^2(\lambda_x - \phi_{x,k}^h) \\ &\quad + C(u_{H,k}^{\text{ms},h}) \sum_{x \in \mathcal{N}} H \|n \cdot A \nabla \phi_{x,k}^h\|_{L^2(\partial \omega_{x,k})}^2 \end{aligned}$$

- 1 Compute multiscale approximation, $u_{H,k}^{\text{ms},h}$.
- 2 Compute local error indicators.
- 3 If the error bound is small enough break.
- 4 Otherwise, decrease h locally if interior indicator is large and increase k locally if boundary indicator is large.
- 5 Go back to 1.

Numerical example

- Let the coarse mesh consist of 32×32 elements.
- Let the fine reference mesh consist of 256×256 elements.
- $f = -1$ in lower left corner ($0 \leq x, y \leq 1/128$) and $f = 1$ in upper right corner, otherwise $f = 0$.
- $A =$



We use a symmetric **DG method** as base for the multiscale method. Local problems are solved using **Neumann boundary conditions**, hanging nodes are allowed, there is a common reference mesh.

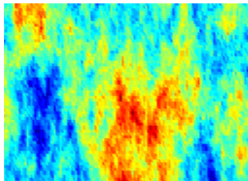


D. Elfverson, E. Georgoulis, and A. Målqvist.

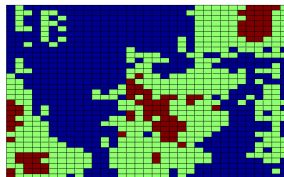
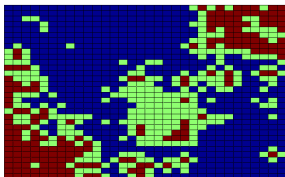
An adaptive discontinuous Galerkin multiscale method for elliptic problems,
Submitted to SIAM MMS.

Numerical example

We start with $h = H/2$ and $k = 2$ in all local problem. In each iteration we refine (divide h by 2) and increase (add 1 to k) 30% of the patches.

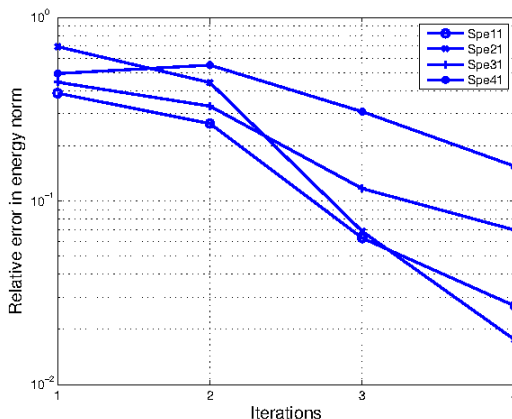


We plot h and k for SPE layer 31 after three iterations.



Numerical example

Convergence of relative error vs. number of iterations.



We note that SPE layer 41 is more difficult, $\max a / \min a \approx 6 \cdot 10^6$ instead of $6 \cdot 10^5$.

Why DG?

Advantage:

- It allows for Neumann conditions on the patches (leading to discontinuous basis functions).
- More flexibility in the adaptively refined local subgrids using hanging nodes.
- Construction of a conservative flux, which is essential in the application area, is easy.
- Can be applied on the coarse scale and combined with CG on the fine scale.

Disadvantage:

- Expensive.
- There is a penalty parameter which needs to be tuned.

Outline

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- 2 Multiscale Method and Convergence
- 3 Full discretization and Numerical Experiments
- 4 Adaptivity
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- 6 Conclusion

Ongoing work

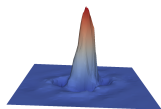
The key is to simplify the computation of the modified basis and to reuse the multiscale basis in the computation.

- 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 $\mathfrak{F}\lambda_x \in V^f$ such that

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

$$V_H^{\text{ms}} = \text{span}(\{\lambda_x - \mathfrak{F}\lambda_x\}), \text{ and } x \in \mathcal{N}.$$



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,

$$\|A^{1/2} \nabla(u - u_H^{\text{ms}})\|_{L^2(\Omega)}^2 \lesssim \alpha^{-1/2} \|H^{1+s} D^s f\|_{L^2(\Omega)} + \alpha^{-1} H \left(\|B\|_{L^\infty(\Omega)} + H \|C - \nabla \cdot B\|_{L^\infty(\Omega)} \right) \|g\|_{H^{-1}(\Omega)},$$

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,

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

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,

$$\begin{aligned} \frac{1}{2} \|u(T) - u_H^{\text{ms}}(T)\|_{\Omega}^2 + \int_0^T \|A^{1/2} \nabla(u - u_H^{\text{ms}})\|_{L^2(\Omega)}^2 dt \\ \lesssim \alpha^{-2} \int_0^T \|H(f - \mathfrak{I}_{\mathcal{T}} f)\|_{L^2(\Omega)}^2 dt. \end{aligned}$$

- 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:

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

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

Outline

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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.
- An adaptive algorithm for automatic tuning of critical method parameters is presented.
- 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 $\mathfrak{S}_{\mathcal{T}} u_{H,k}^{\text{ms},h}$, 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.