NordForsk project meeting

Multiscale problems and uncertainty

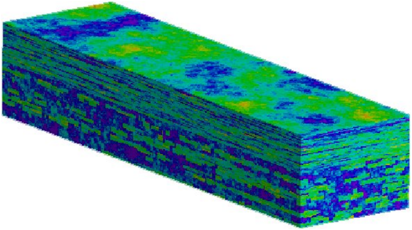
Axel Målqvist

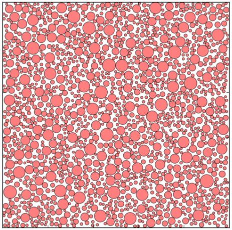
Chalmers and University of Gothenburg

Oslo 2015-06-03

Multiscale problems with uncertainty

Applications such as





- ▹ flow in a porous medium
- ▹ composite materials

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

Major challenge: Features on multiple scales and data uncertainty.

Focus of my research

Multiscale methods:

- construction of numerical methods for efficient solution of multiscale problems,
- convergence analysis based on finite element a priori error estimation techniques,
- application to semi-linear, time dependent, and (linear and non-linear) eigenvalue problems.

Uncertainty quantification:

- development of algorithms for efficient solution of PDE's with multiple realisations of the data (Monte Carlo setting),
- error analysis and adaptivity with respect to both statistical and numerical errors,

My research group

Axel Målqvist, Göteborg, Assoc. Prof., Mathematics

Postdoc:

Tony Stillfjord, Göteborg, Time dep. PDE and splitting, 2015-2017

Ph.D. students:

Daniel Elfverson, Uppsala, Multiscale and UQ, 2011-2015
Fredrik Hellman, Uppsala, Multiscale and UQ, 2012-
Anna Persson, Göteborg, Time dep. ms problems, 2013-
Gustav Kettil, Göteborg, Simulation of paper, 2014-

M.Sc. student

Robert Forslund, Multiscale, 2015

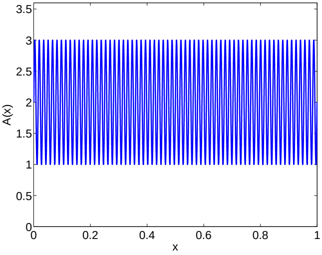
Motivation for multiscale techniques

Poisson's equation

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

where A has rapid oscillations.

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



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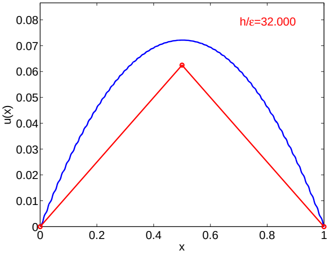
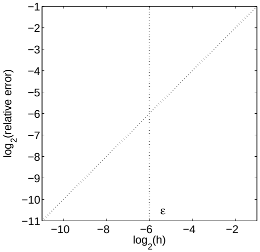


solution and P1-FEM-approximation



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

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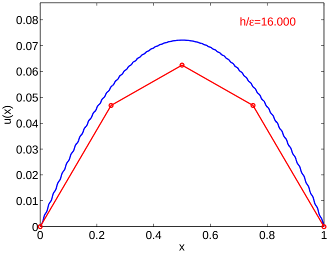

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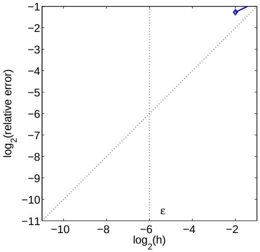

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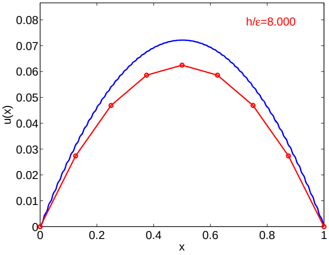

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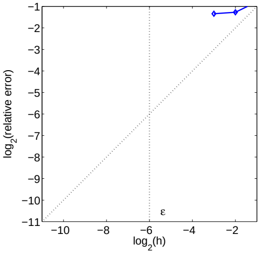

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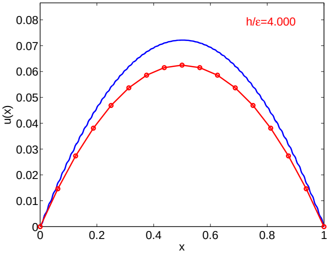

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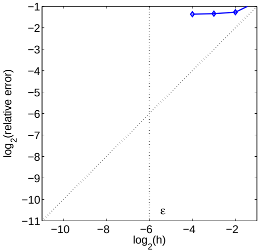

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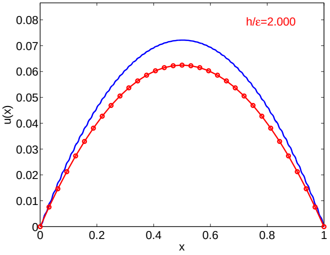

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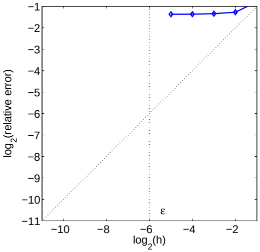

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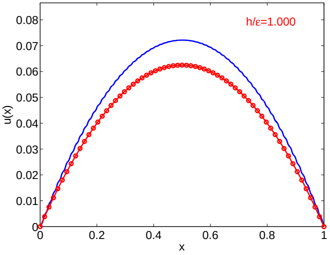

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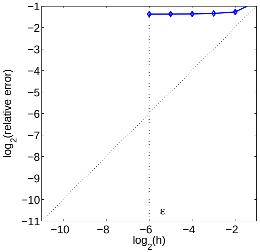

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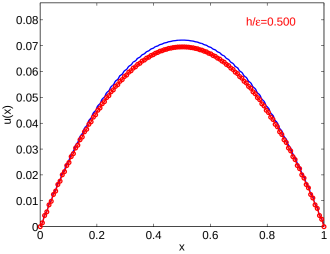

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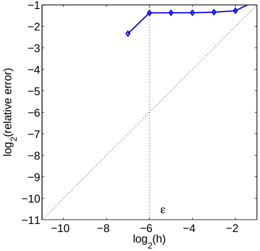

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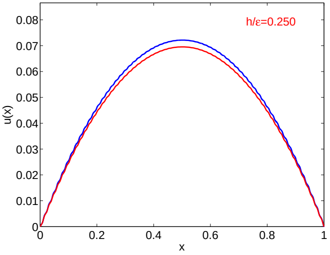

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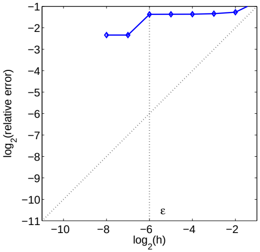

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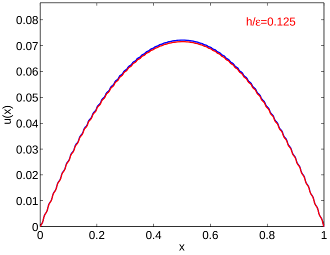

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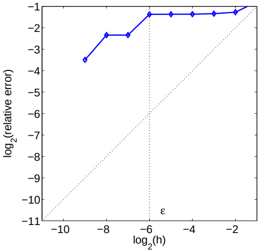

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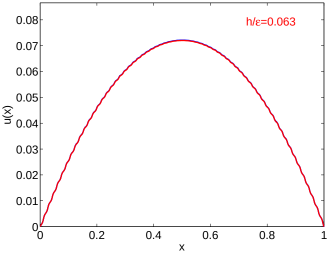

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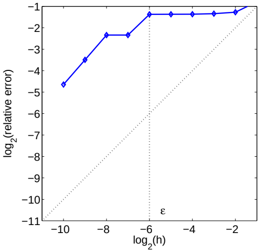

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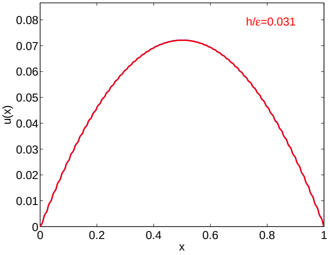

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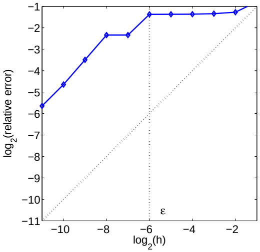

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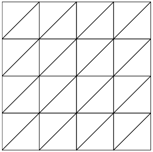
Conclusion

- Fine scale features have to be resolved even to get coarse solution behavior right (both H^1 and L^2 errors are large).
- Resolution of the fine scales by a uniformly refined mesh is very computationally expensive.
- We want to find an alternative basis better suited for the problem.

Standard FE decomposition

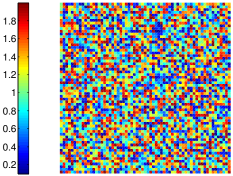
- Coarse FE mesh with parameter H
- Piecewise linear continuous FE space V_H
- $P_{L^2(\Omega)} : V \to V_H$, $V^{\mathrm{f}} := \{v \in V \mid P_{L^2(\Omega)} v = 0\}$



Decomposition

$$V = V_H \oplus V^{\mathrm{f}} \quad \text{with} \int_\Omega v_H \cdot v_f \, dx = 0$$

Example:



rough coefficient

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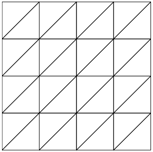

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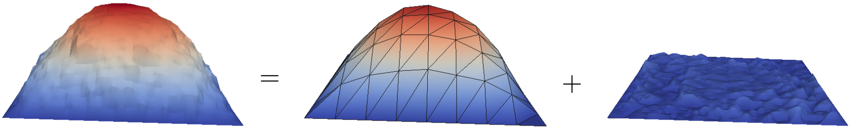
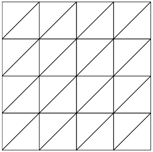


$u \in V$ = $u_H \in V_H$ + $u^{\mathrm{f}} \in V^{\mathrm{f}}$

Orthogonal multiscale decomposition

- We keep $V^{\mathrm{f}} := \{v \in V \mid P_{L^2(\Omega)} v = 0\}$ find V_H^{ms}
- Start from V_H and add fine scale corrections in V^{f}
- so that V_H^{ms} is orthogonal w.r.t. the bilinear form



Decomposition

$$V = V_H^{\mathrm{ms}} \oplus V^{\mathrm{f}} \quad \text{with} \quad \int_\Omega A \nabla v_H^{\mathrm{ms}} \cdot \nabla v^f \, dx = 0$$

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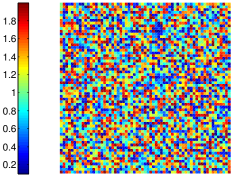

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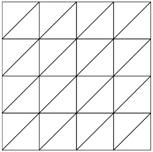

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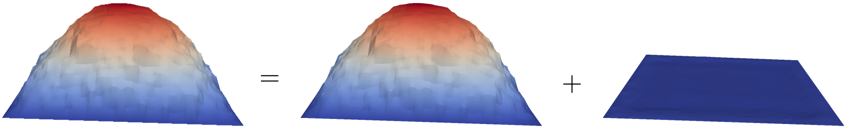

$u \in V$ $=$ $u_H^{\mathrm{ms}} \in V_H^{\mathrm{ms}}$ $+$ $u^{\mathrm{f}} \in V^{\mathrm{f}}$

Computing a basis

Let $V_H = \text{span}\,\{\lambda_x \mid x \in \mathcal{N}\}$ and further let, $\phi_x \in V^{\mathrm{f}}$ solve

$$\int_\Omega A\nabla(\lambda_x - \phi_x)\cdot\nabla w\,dx = 0, \quad \text{for all } w \in V^{\mathrm{f}}.$$

Multiscale FE space

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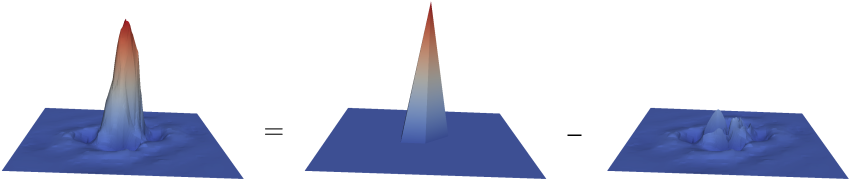

$\lambda_x - \phi_x \in V_H^{\mathrm{ms}}$ = $\lambda_x \in V_H$ − $\phi_x \in V^{\mathrm{f}}$

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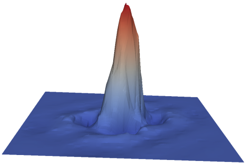

$\lambda_x - \phi_x \in V_H^{\text{ms}}$

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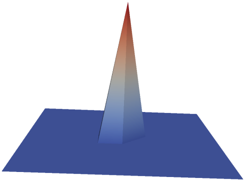
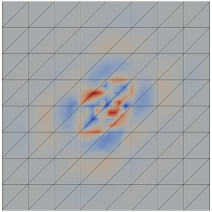


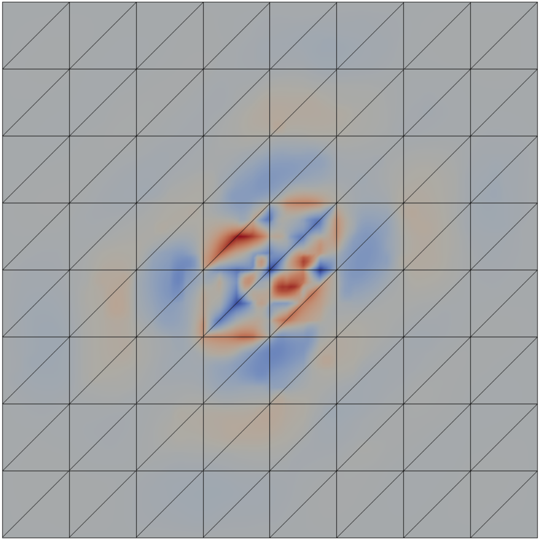
$\lambda_x \in V_H$

−



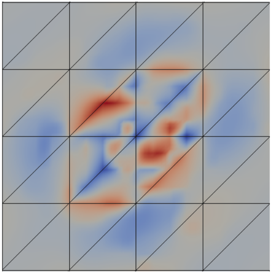
$\phi_x \in V^{\text{f}}$

Computing a basis



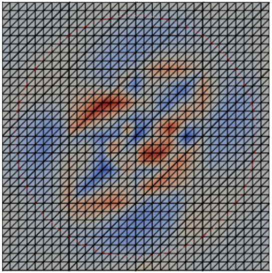
We have proven exponential decay of $\lambda_x - \phi_x$!

Computing a basis



This allows us to truncate to a patch.

Computing a basis



This allows us to truncate to a patch and fine scale discretization.

Computing the multiscale approximation

Multiscale approximation: $u_H^{\text{ms}} \in V_H^{\text{ms}}$ satisfies

$$\int_\Omega A \nabla u_H^{\text{ms}} \cdot \nabla v \, dx = \int_\Omega f \cdot v \, dx \quad \text{for all } v \in V_H^{\text{ms}}$$

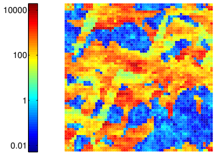
- We have proven error bound (using $k = \log(1/H)$ layers):

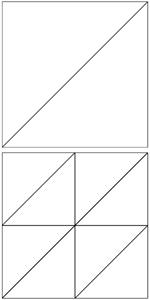
$$\|\nabla(u - u_H^{\text{ms}})\| \leq CH\|f\|,$$

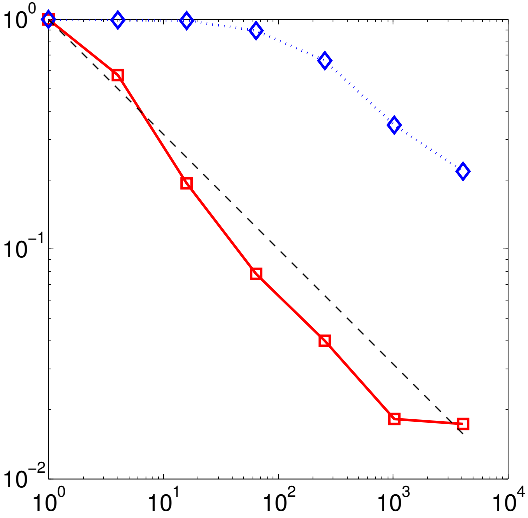
  where $\|v\|^2 = \int_\Omega v^2 \, dx$ and C is independent on variations in A.
- Note that for the standard FEM with $A = A(\frac{x}{\epsilon})$ we have,

$$\|\nabla(u - u_H)\| \leq C\frac{H}{\epsilon}\|f\|.$$

Numer. exp. Poisson, $f \in L^2$







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

$\|\nabla(u_h - u^{\mathrm{ms},h}_{H,k})\|$ vs. #dof

Quantile estimation

Poisson equation with random diffusion $A(\omega)$ and given boundary data: Given $\omega \in \Omega$ find $u = u^0 + g$ with $u^0 \in H^1_0(D)$ such that,

$$\int_D A(\omega)\nabla u \cdot \nabla v \, dx = 0, \quad \forall v \in H^1_0(D).$$

We want to compute a functional e.g. $q(u) = \int_\Gamma n \cdot A(\omega)\nabla u \, ds$, where $\Gamma \subset \partial\Omega$.

Given p we want to compute a quantile x such that

$$P(q(u) < x) = F(x) = p,$$

e.g. with 95% probability the flux is less than x.

Uncertainty quantification

Quantile estimation

Poisson equation with random diffusion $A(\omega_i)$ and given boundary data: Given $\{\omega_i\}_{i=1}^n \in \Omega$ find $u_i^h = (u_i^h)^0 + g$ with $(u_i^h)^0 \in V^h$ such that,

$$\int_D A(\omega_i)\nabla u_i^h \cdot \nabla v \, dx = 0, \quad \forall v \in V^h.$$

We use Monte Carlo sampling and FEM to get a computable empirical cdf,

$$F_n^h(x) = \frac{\#\{i : q(u_i^h) < x\}}{n} \approx F(x) = P(q(u) < x).$$

The approximate quantile is given by $x_n^h = \inf\{x : F_n^h(x) \geq p\}$.

We want to estimate the error $x - x_n^h$ in terms of n and h.

A posteriori error analysis

From statistics we have $|F(y) - F_n(y)| \leq \mathcal{E}_{\text{stat}}(p^*, n, y)$ with prob. p^*.

From numerical analysis we have, $|q(u_i) - q(u_i^h)| \leq \mathcal{R}(\omega_i, u_i^h)$,

$$\frac{\#\{i : q(u_i^h) + \mathcal{R}(\omega_i, u_i^h) < x\}}{n} \leq \begin{matrix} F_n(y) \\ F_n^h(y) \end{matrix} \leq \frac{\#\{i : q(u_i^h) - \mathcal{R}(\omega_i, u_i^h) < x\}}{n}$$

$$|F(y) - F_n^h(y)| \leq |F_n^+(y) - F_n^-(y)| + \mathcal{E}_{\text{stat}}(p^*, n, y) := \mathcal{E}_{\text{tot}},$$

with probability p^*.

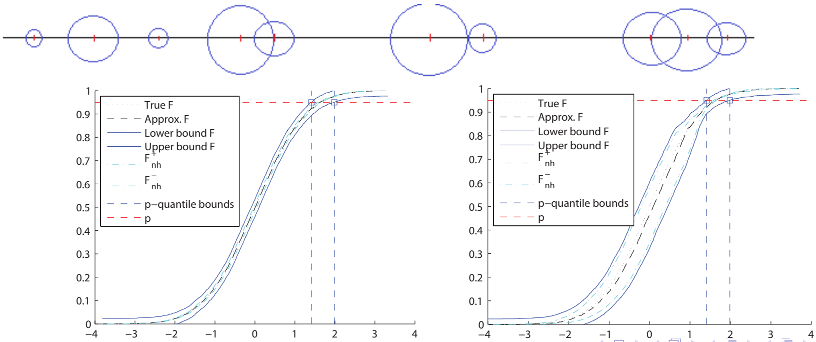
Given a computable bound of the error in the cdf we get a bound for the quantile,

$$\inf\{y : F_n^h(y) + \mathcal{E}_{\text{tot}} \geq p\} \leq x \leq \inf\{y : F_n^h(y) - \mathcal{E}_{\text{tot}} \geq p\}$$

Adaptivity and selective refinement

We have computable bounds for $x^- \leq x \leq x^+$ in terms of h and n which can be used to automatically choose these parameters.

Furthermore, in order to compute e.g. $x_n^h = \inf\{x : F_n^h(x) \geq p\}$ we can allow for much larger h for samples that are far form x.



Expectations

- Go beyond model problems.
- Make the results available to a wide audience.
- Strong connection between analysis, implementation, and applications.

Areas were I can contribute:

- Systematic approach to a posteriori error analysis and adaptivity for PDE's with data uncertainty.
- Goal oriented both with respect to spatial functionals and statistical quantities (quantiles, failure probability)