Progress in the SSF project "CutFEM, Geometry, and Optimal design"

Computer simulation of multiscale problems

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University of Gothenburg and Uppsala University

Umeå 2015-05-20

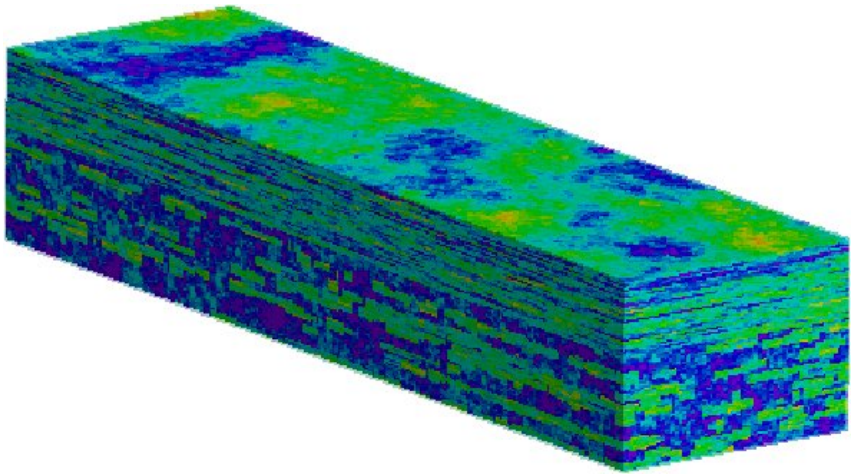
Research group and Outline

My research group consists of:
Daniel Elfverson, Uppsala, Multiscale and UQ, 2011-2015
Fredrik Hellman, Uppsala, Multiscale and UQ, 2012-2017
Anna Persson, Göteborg, Time dep. ms problems, 2013-2018
Gustav Kettil, Göteborg, Simulation of paper, 2014-2016
Tony Stillfjord, Göteborg, Time dep. PDE and splitting, 2015-2017
Support from SSF project 2016-2018.

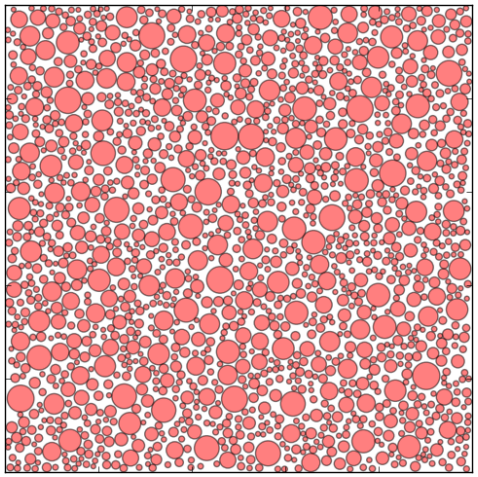
- Introduction to Localized Orthogonal Decomposition techniques for solving multiscale problems (Axel)
- Application to eigenvalue problems (Axel)
- Application to problems posed on complex geometry (Daniel)
- Recent development and openings for collaboration (Axel)

Multiscale problems

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 in space and time.

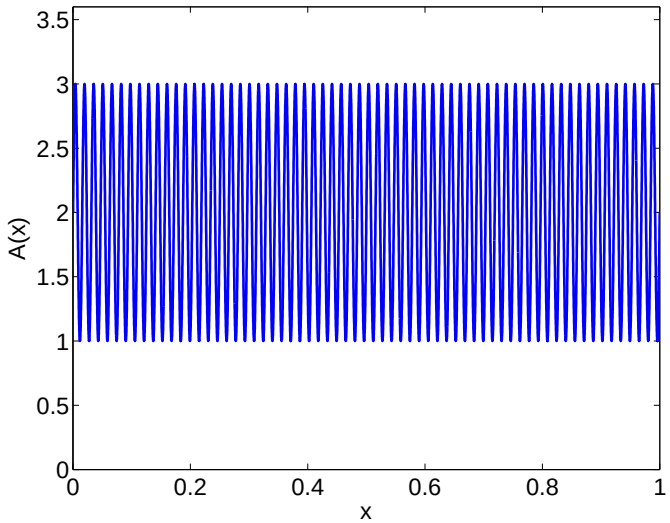
Motivation for multiscale techniques

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



oscillatory coefficient

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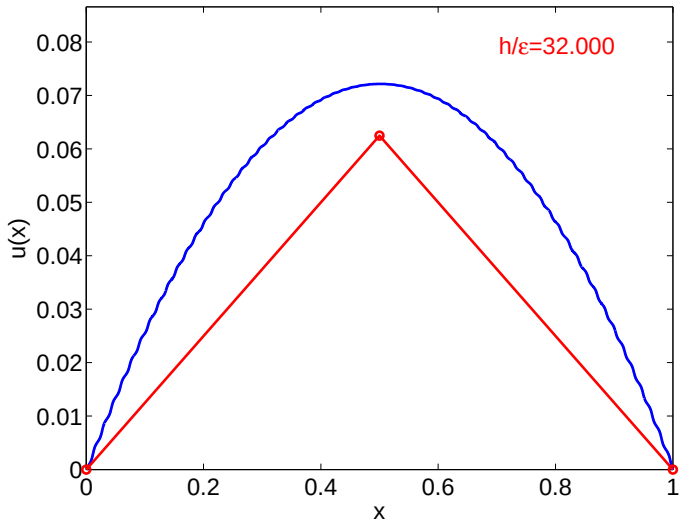
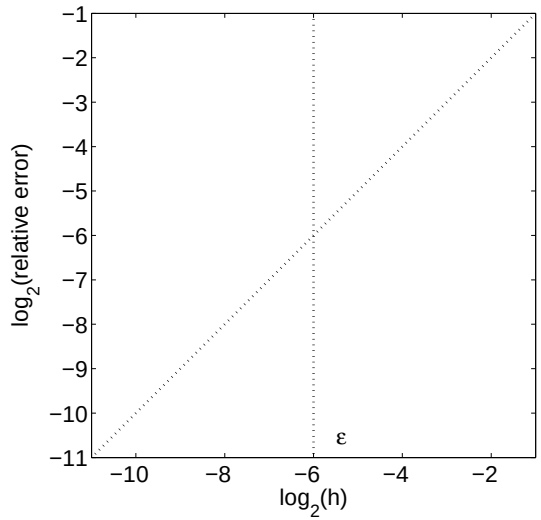


solution and P1-FEM-approximation



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

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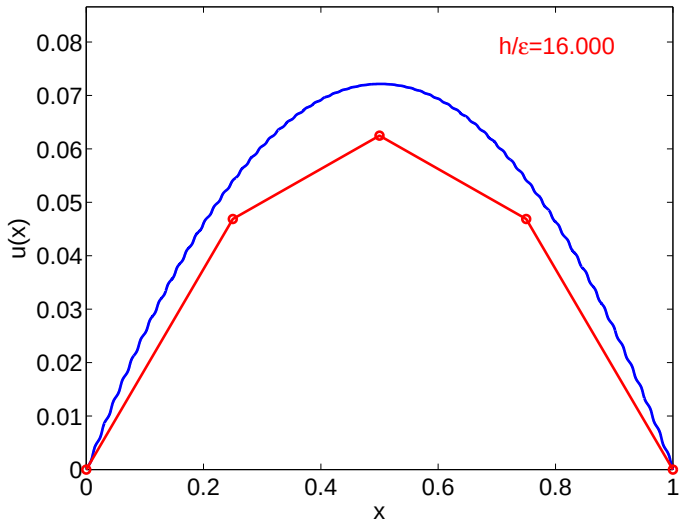

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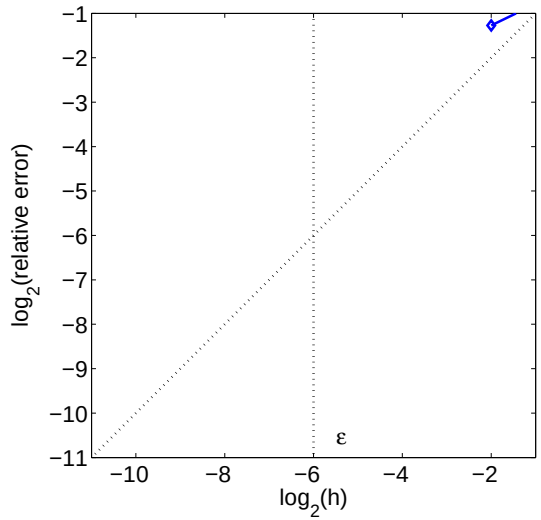

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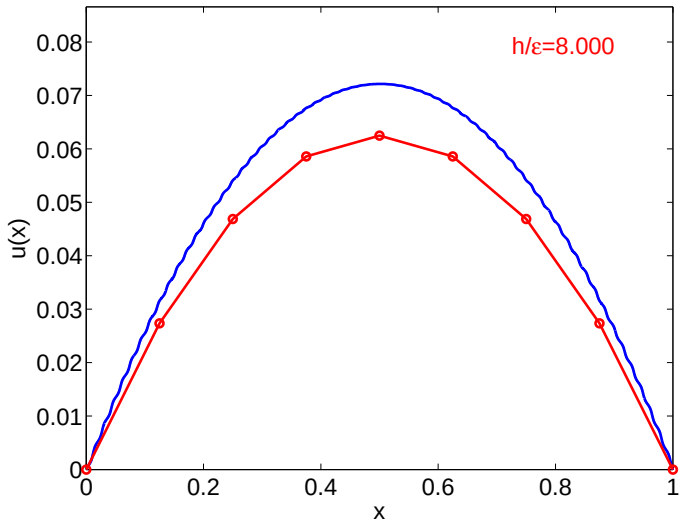

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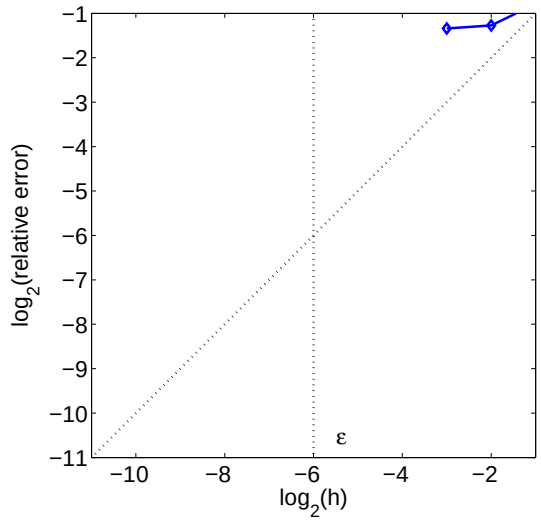

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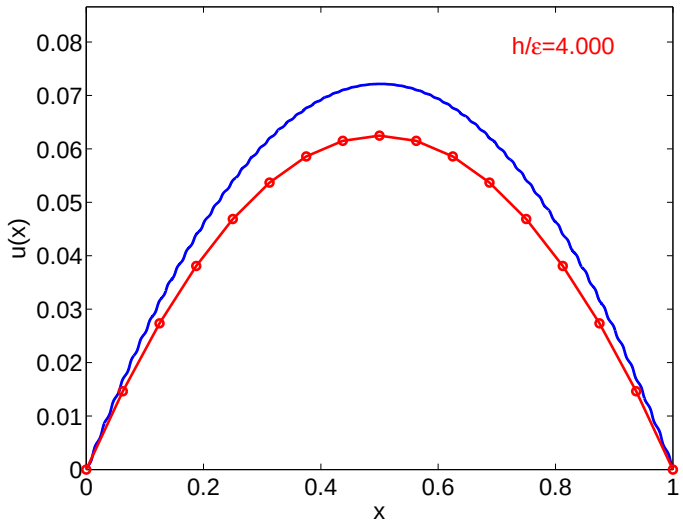

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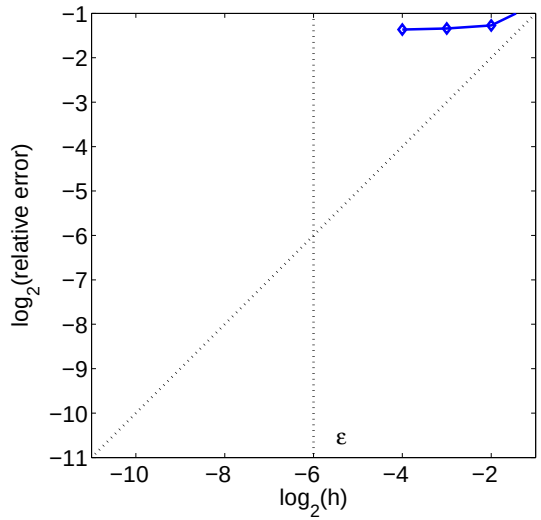

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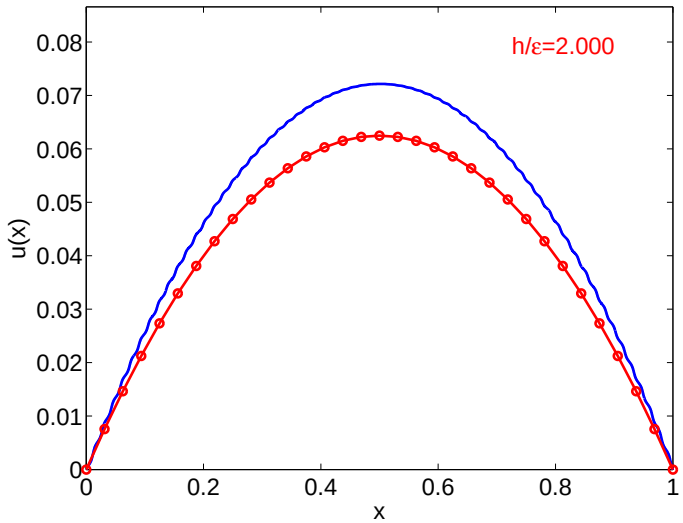

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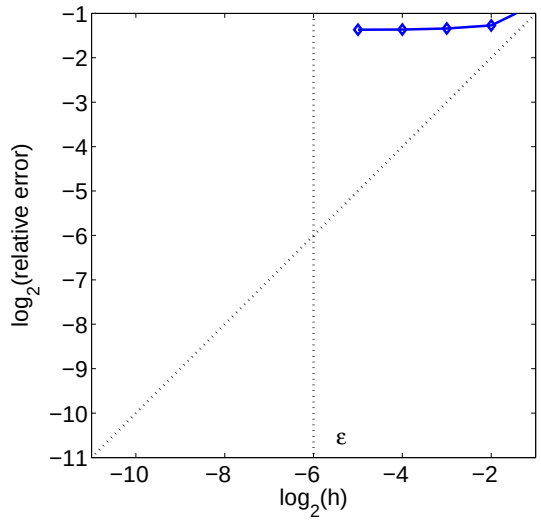

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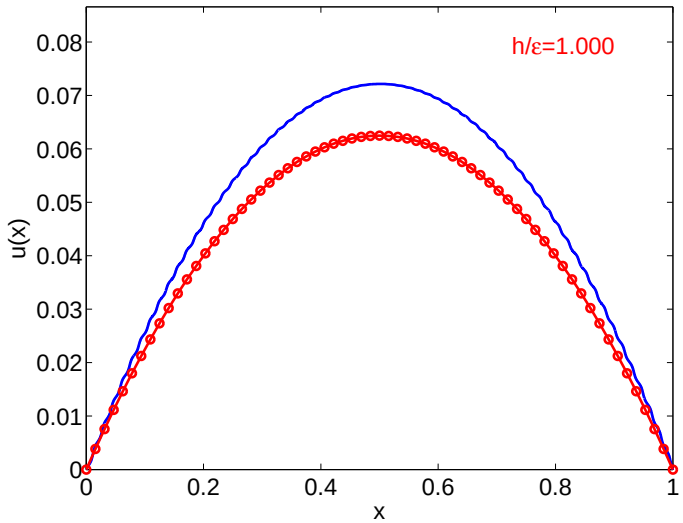

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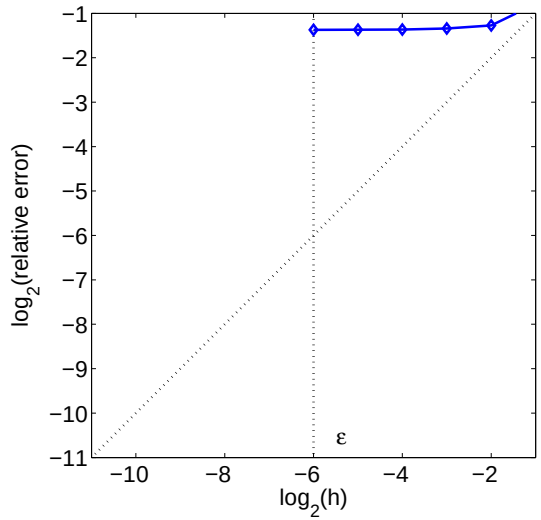

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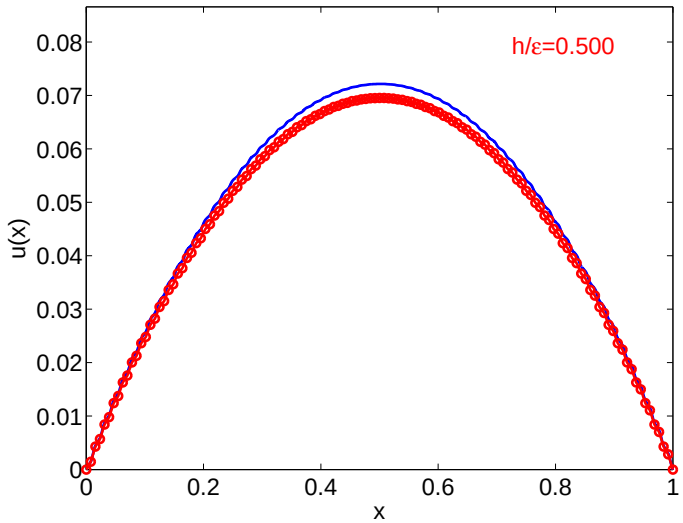

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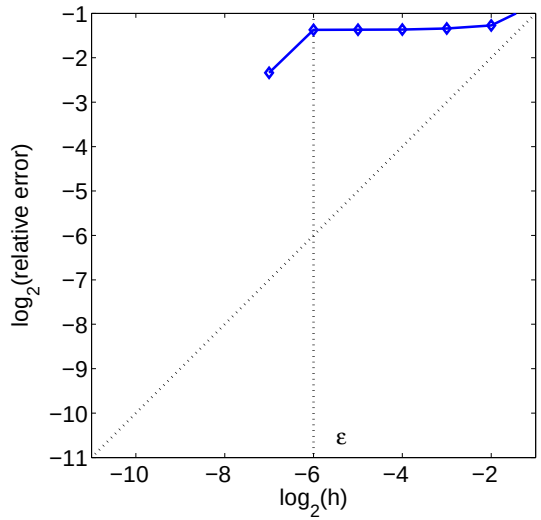

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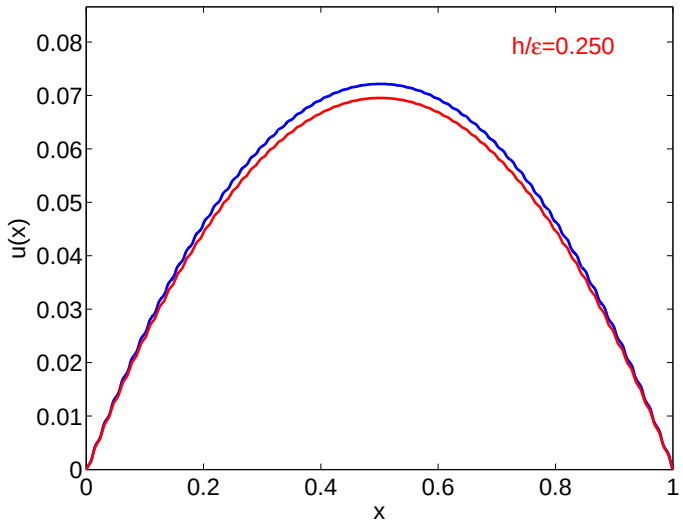

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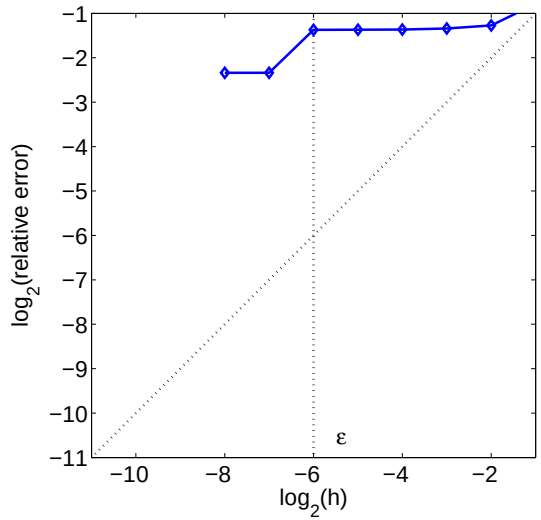

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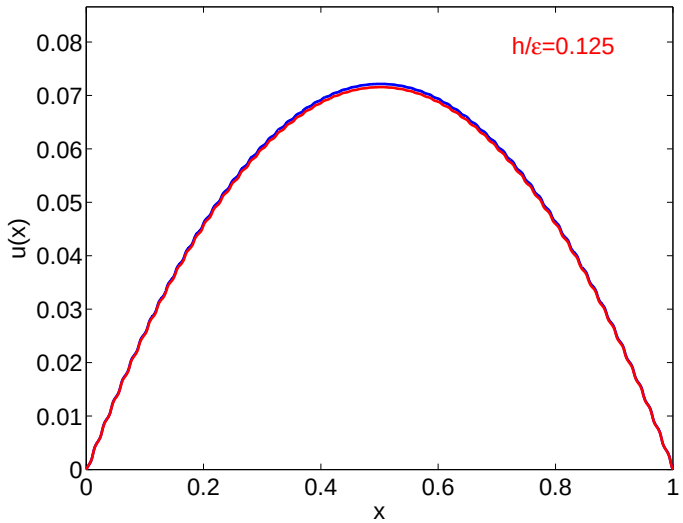

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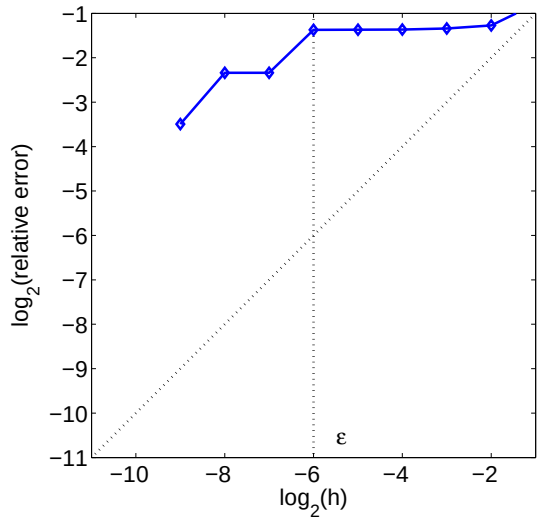

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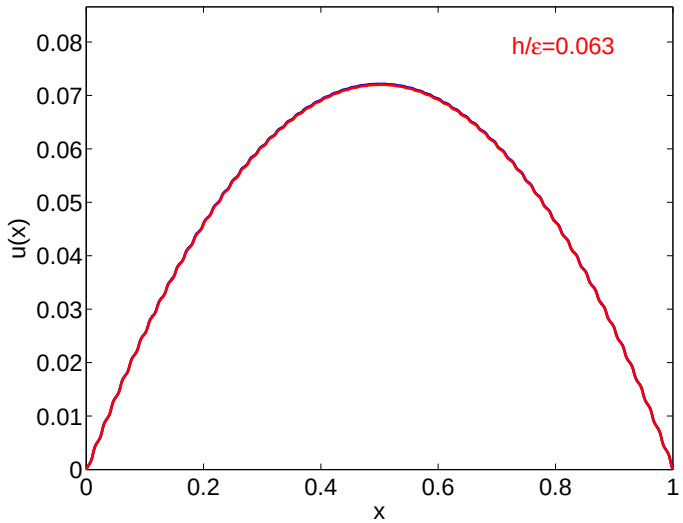

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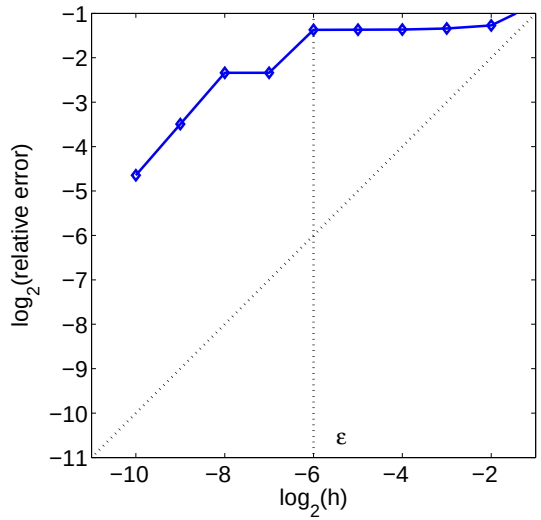

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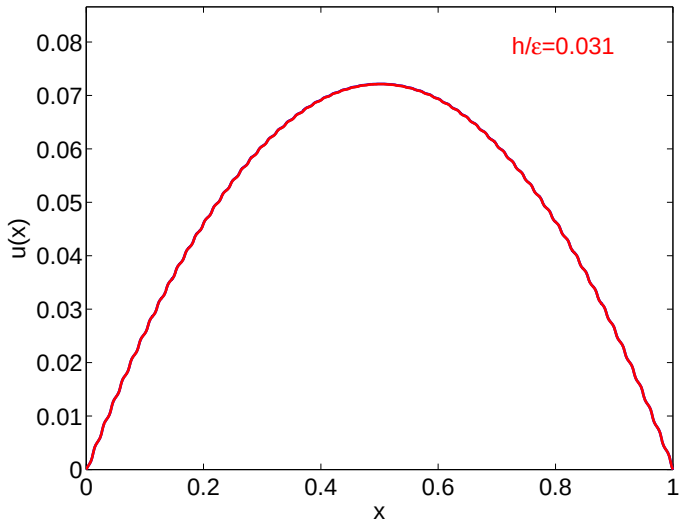

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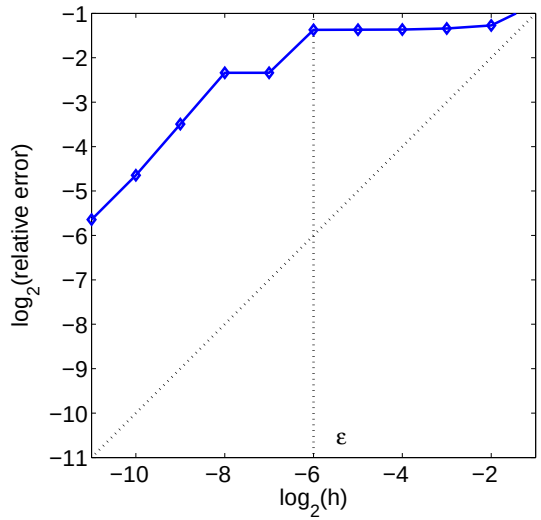

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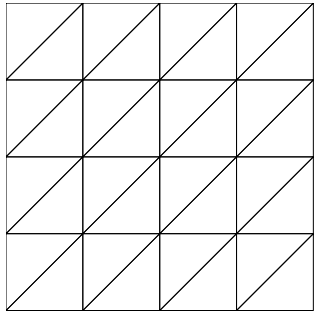
Conclusion

- 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 uniform mesh is very computationally expensive.
- Local mesh refinement is not an option.
- The standard basis does not seem to be suitable for this problem.

Standard FE decomposition

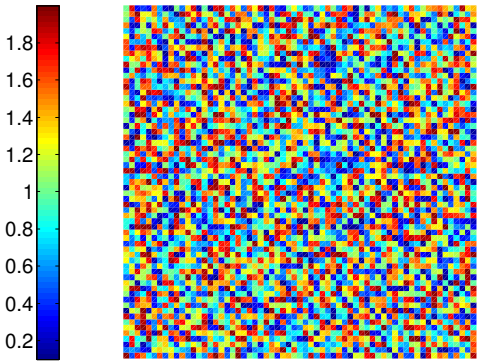
- Coarse FE mesh with parameter H
- Piecewise linear continuous FE space V_H
- $\mathfrak{I}_{\mathcal{T}} : V \to V_H$ interpolation operator



Decomposition

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

Example:



rough coefficient

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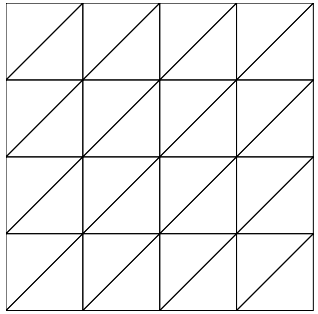

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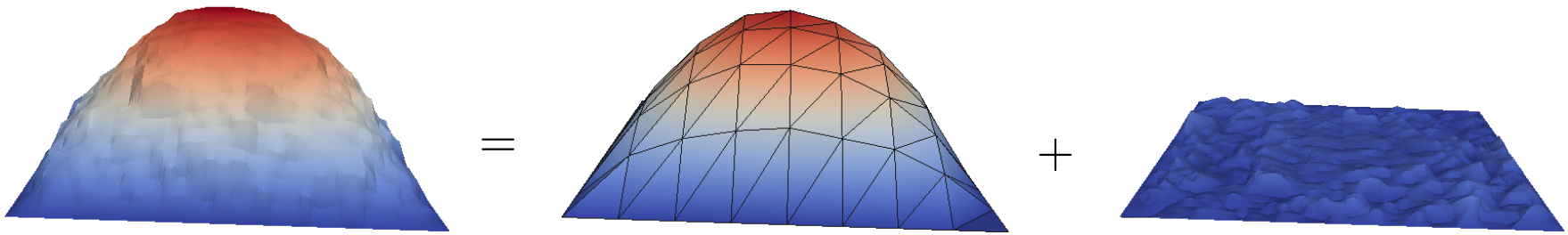
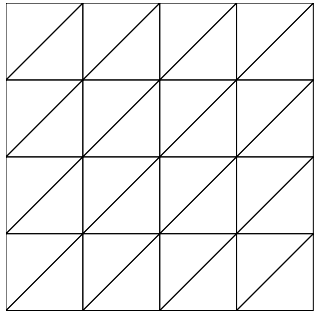


$u \in V$ $\quad$ $u_H \in V_H$ $\quad$ $u^{\mathrm{f}} \in V^{\mathrm{f}}$

Orthogonal multiscale decomposition

- Let $\dim(V_H^{\text{ms}}) = \dim(V_H)$
- Start from V_H and add fine scale corrections in V^{f}
- $\forall\ v_H^{\text{ms}} \in V_H^{\text{ms}}, v_f \in V^{\text{f}}$ holds $\int_\Omega A\nabla v_H^{\text{ms}} \cdot \nabla v_f\, dx = 0$



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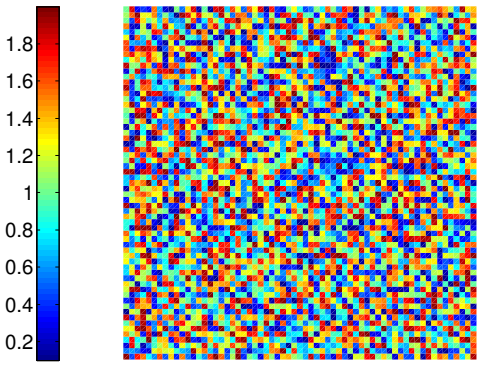

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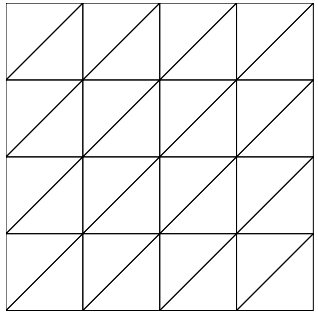

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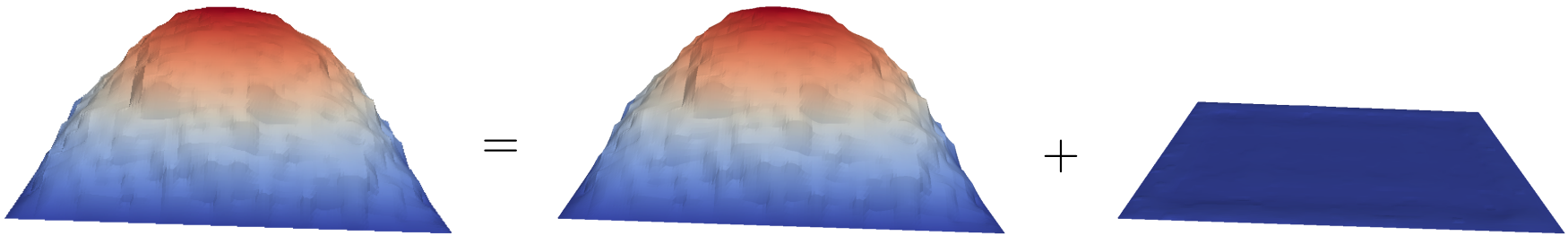

$u \in V$ $\qquad$ $u_H^{\text{ms}} \in V_H^{\text{ms}}$ $\qquad$ $u^{\text{f}} \in V^{\text{f}}$

Computing a basis

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

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

Multiscale FE space

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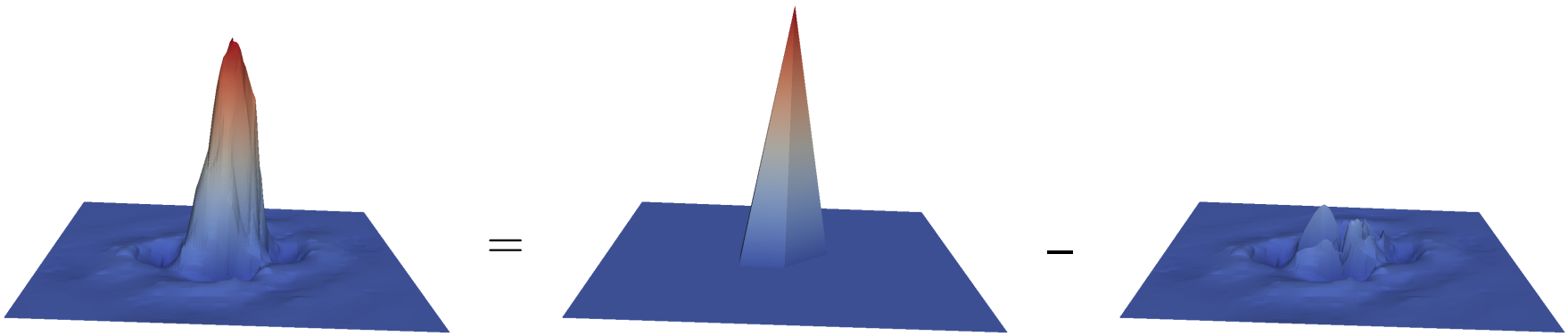

$\lambda_x - \phi_x \in V_H^{\text{ms}}$ $\quad = \quad$ $\lambda_x \in V_H$ $\quad - \quad$ $\phi_x \in V^{\text{f}}$

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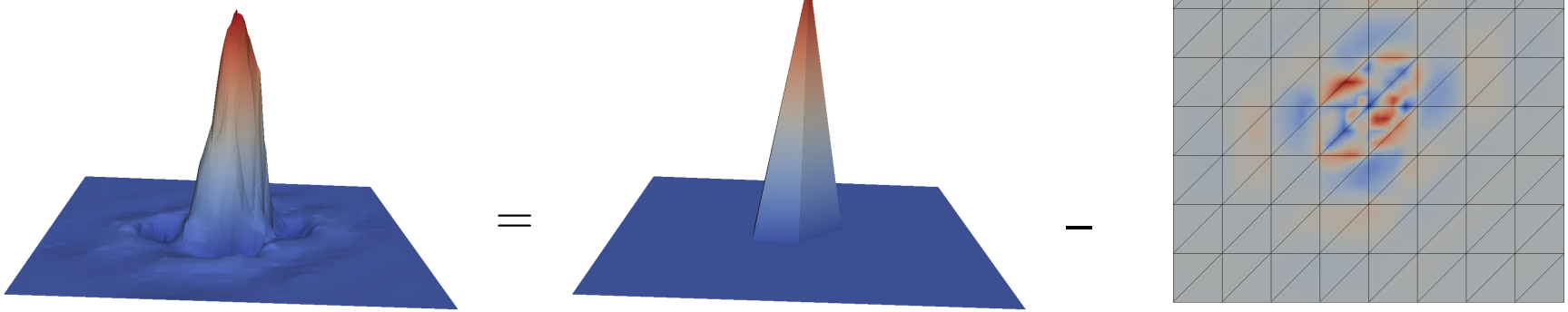
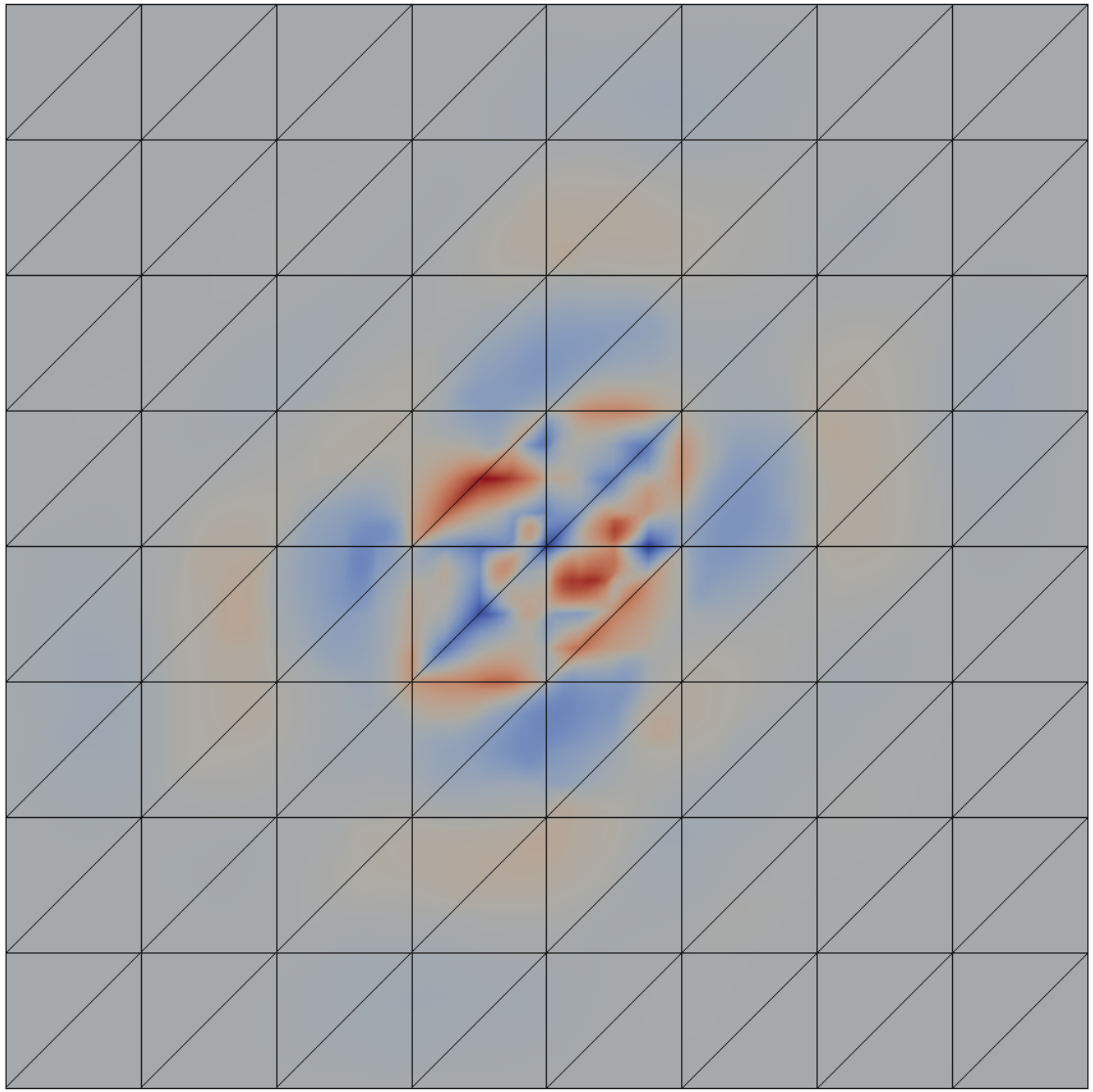
$$V_H^{\mathrm{ms}} = \operatorname{span}\{\lambda_x - \phi_x \mid x \in \mathcal{N}\}$$

Example:



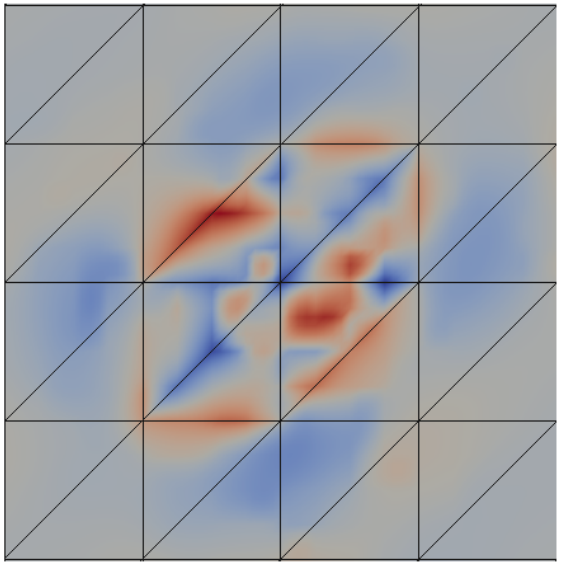
$\lambda_x - \phi_x \in V_H^{\mathrm{ms}}$ $\quad = \quad$ $\lambda_x \in V_H$ $\quad - \quad$ $\phi_x \in V^{\mathrm{f}}$

Computing a basis



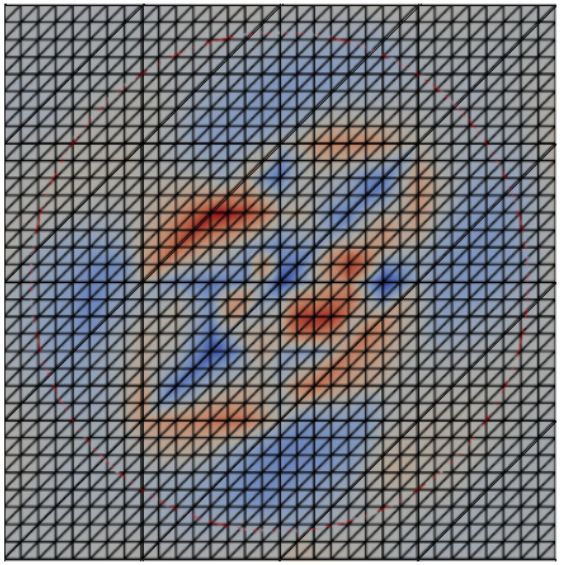
We have proven exponential decay of $\lambda_x - \phi_x$!

Computing a basis



This allows us to truncate to a patch.

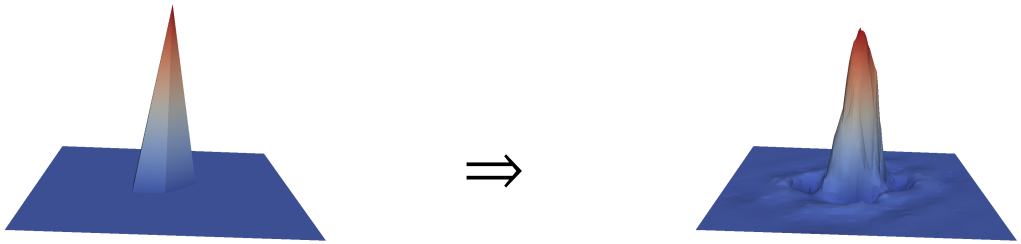
Computing a basis



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

Computing a basis

Localized patch with refined mesh gives computable basis functions



- The multiscale basis functions are computed by solving the PDE on local patches.
- The basis functions are totally independent, leading to trivial parallelization.
- Exponential decay has been proven and is crucial.
- Remember $\dim(V_H^{\text{ms}}) = \dim(V_H)$.

Computing the multiscale approximation

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

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

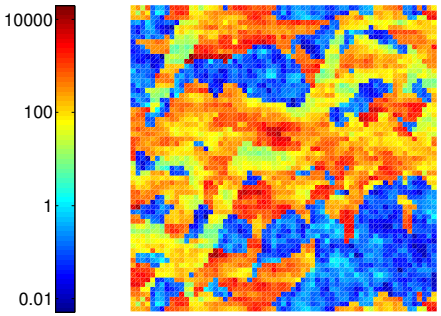
- We have proven error bound (using $k = \log(1/H)$ layers):

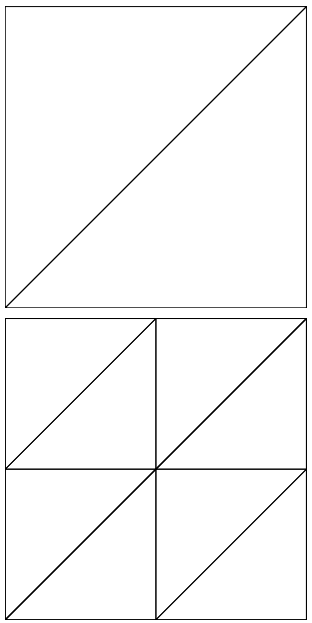
$$\|\nabla(u - u_H^{\text{ms}})\| \leq CH\|f\|,$$

  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,

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

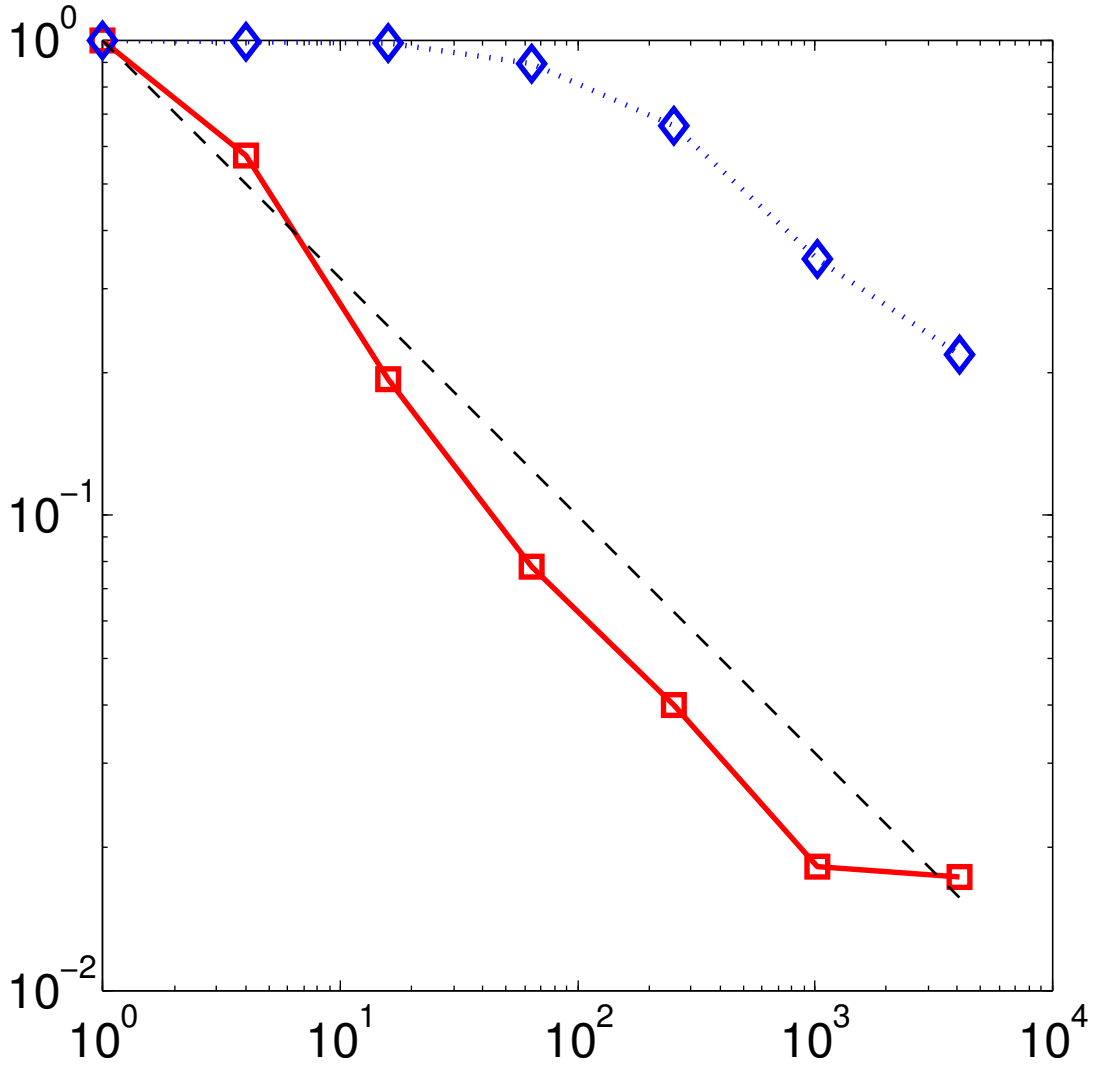
Numer. exp. (Poisson, $f \in L^2(H)$, $f \in H_0^1(H^2)$!)





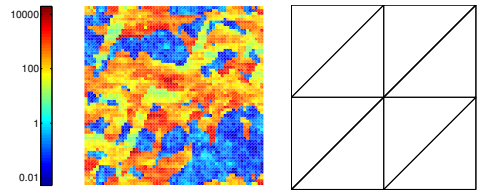
$H = 2^{-1}, 2^{-2}, \ldots, 2^{-7}$

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



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

Numer. exp. (linear eigenvalue problem, H^4)



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

The quadratic eigenvalue problem

Consider discretized structure with damping,

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

where $K_{ij} = (A\nabla\phi_j, \nabla\phi_i)$ is stiffness, $C_{ij} = c(\phi_j, \phi_i)$ is damping, and $M_{ij} = (\phi_j, \phi_i)$ is mass matrix.

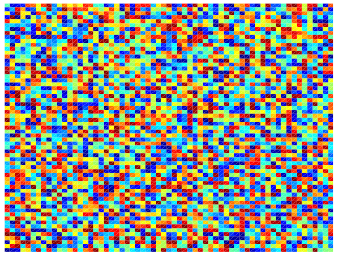
Linearization: $(y = \lambda x)$

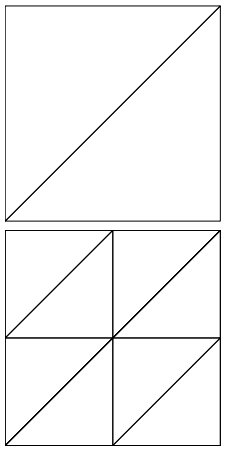
$$Ax := \begin{bmatrix} K & 0 \\ 0 & M \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \lambda \begin{bmatrix} -C & -M \\ M & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} := \lambda Bx,$$

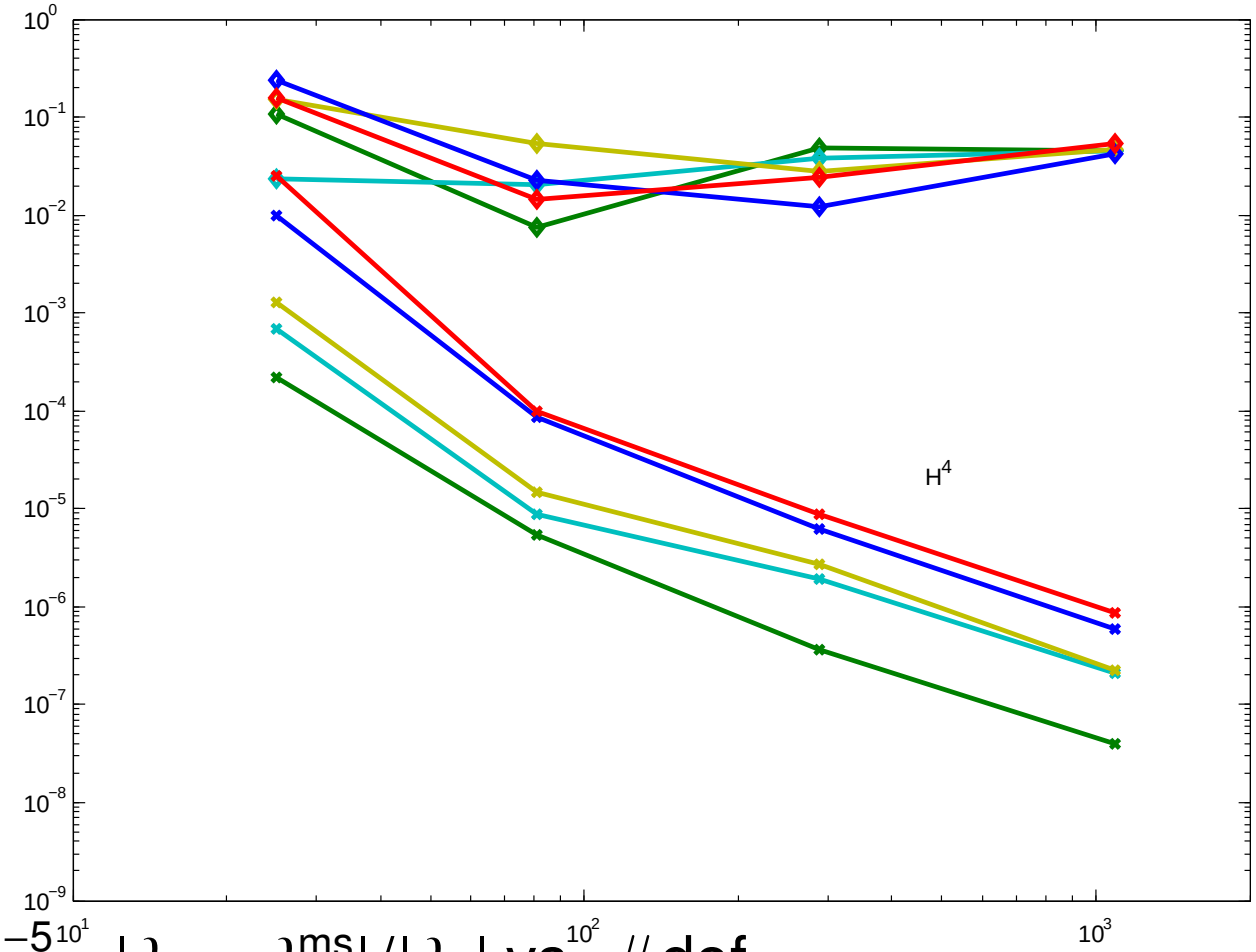
Note that $T = A^{-1}B$ has eigenvalues λ^{-1}. T is not symmetric (even if C is), it is compact but not necessarily in the limit $h \to 0$.

The analysis is very different from symmetric case. Semi-simple eigenvalues are ok but defective leads to unknown constants.

Numerical experiment







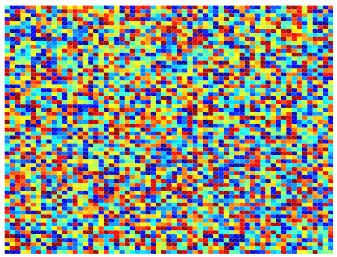
$H = 2^{-1}, 2^{-2}, \ldots, 2^{-5}$

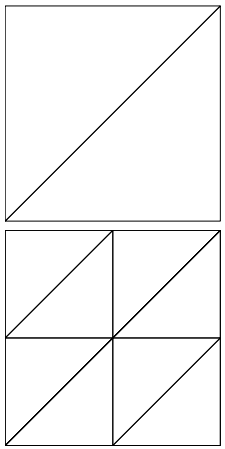
$h = 2^{-6}$, $k = \infty$

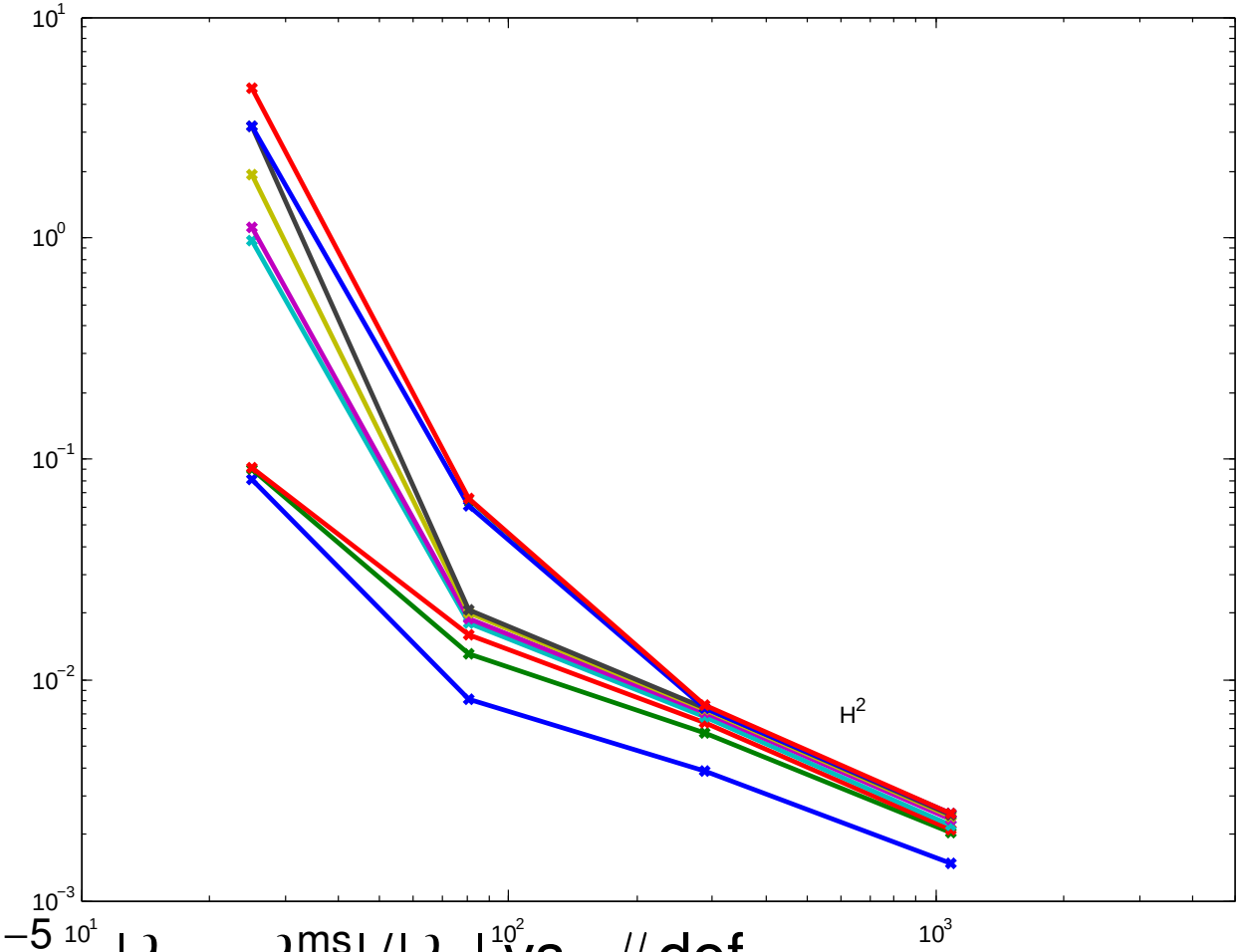
$|\lambda_h - \lambda_H^{\text{ms}}|/|\lambda_h|$ vs. #dof

A (pic), $c(u, v) = \int_\Omega (1 + sin(10x))u\,v\,dx$

Numerical experiment







$H = 2^{-1}, 2^{-2}, \ldots, 2^{-5}$ $|\lambda_h - \lambda_H^{\text{ms}}|/|\lambda_h|$ vs. #dof

$h = 2^{-6}$, $k = \infty$

$$\pi c(u, v) = \int_\Omega (atan(10x - 5) + \tfrac{\pi}{2}) A \nabla u \nabla v \, dx$$

Relevant papers

Some papers relevant for the SSF project (work package D):

- Poisson P1, M. & Peterseim, Math. Comp., 2014.
- Poisson DG, E., Georgoulis, M., & Petersiem, SINUM, 2013.
- Linear Eig., M. & Peterseim, Numer. Math. 2015.
- Gross-Pitaevskii, Henning, M., & Peterseim, SINUM, 2014.
- Helmholtz, Peterseim, two preprints

LOD is applicable when: The diffusion is present and lower order terms are not dominating.

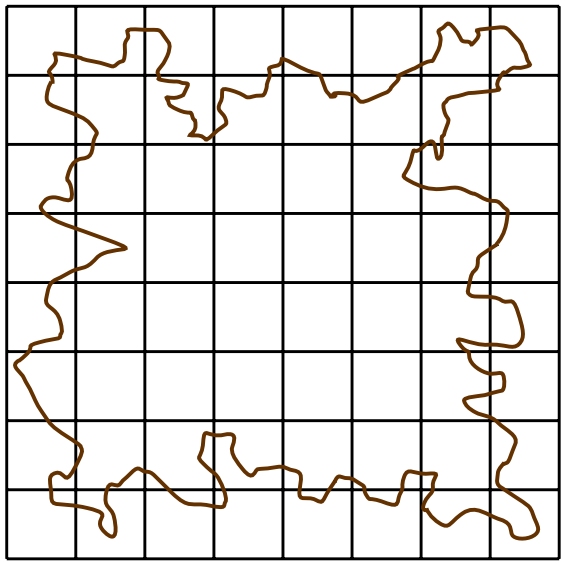
LOD is efficient when: basis can be reused many times in the calculation (nonlinear iteration, time stepping, ...).

LOD – complex geometry

Consider the Poisons equation

$$\begin{aligned} -\Delta u &= f && \text{in } \Omega, \\ \nu \cdot \nabla u &= -\kappa u && \text{on } \Gamma_R, \\ u &= 0 && \text{on } \Gamma_D, \end{aligned}$$

where Γ_D and Γ_R are not resolved by the mesh



Objective

Construct a multiscale method for complicated geometries with the following properties:

- No pre-asymptotic effect
- Linear convergence without resolving the boundary
- Conditioning is independent of how the boundary cut the mesh
- Only enrich the coarse finite element space in the vicinity of the boundary

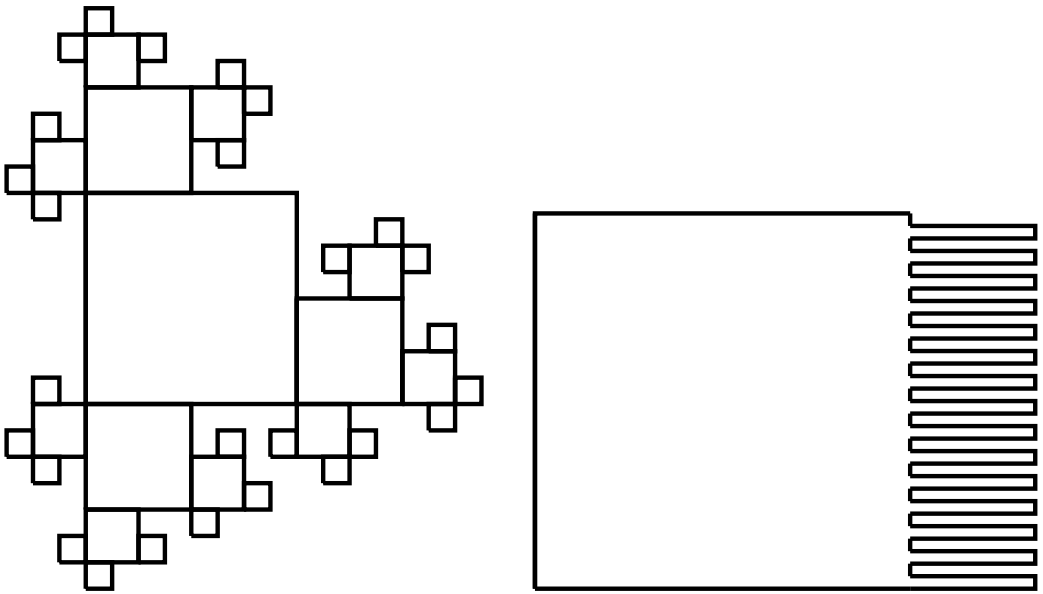
Poincaré-Friedrich inequality

Difficulties: We need a inequality of the type

$$\inf_{c\in\mathbb{R}} \|u - c\|_{L^2(\omega)} \leq C(\omega)\mathrm{diam}(\omega)\|\nabla u\|_{L^2(\omega)}$$

where

- $C(\omega)$ is bounded independent of $\mathrm{diam}(\omega)$



Error analysis

- Let ω_Γ be a vicinity of the complicated boundary

Theorem (Locally enriched LOD method)

Given that $u \in H^1_{\Gamma_D} \cap H^2(\Omega \setminus \omega_\Gamma)$ *and that* $u_H^\Gamma \in V_H^{\Gamma,L}$ *is the LOD solution, then*

$$|||u - u_H^{LOD}|||_h \lesssim \|\nabla(u - \mathfrak{I}_h u)\|_{L^2(\omega_\Gamma)} + H|u|_{H^2(\Omega\setminus\omega_\Gamma)} + H\|f\|_{L^2(\omega_\Gamma)} + H^{-1}(L)^{d/2}\gamma^L\|f\|_{L^2(\Omega)}$$

holds. The condition number scale as $\kappa \lesssim H^{-2}$.

- $\mathfrak{I}_h u$: interpolation operator on the fine mesh
- L: Number of layers
- $0 < \gamma < 1$: depends on the Poinaré-Friedrich constant

Error analysis

- Choose $L = \lceil C \log(H^{-1}) \rceil$,

Theorem (Locally enriched LOD method)

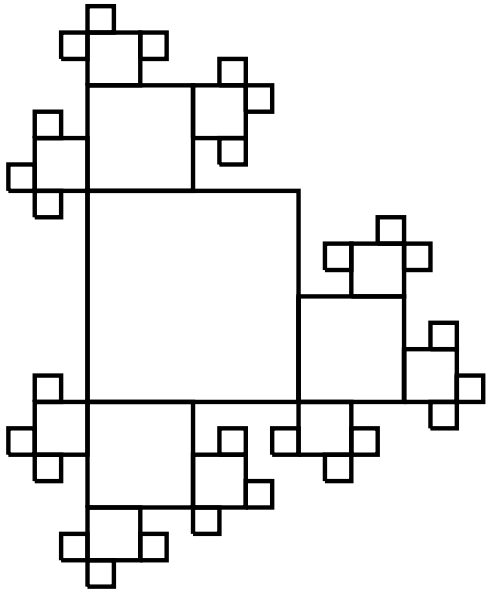
Given that $u \in H^1_{\Gamma_D} \cap H^2(\Omega \setminus \omega_\Gamma^{k-1})$ *and* $u_H^\Gamma \in V_H^{\Gamma,L}$, *then*

$$|||u - u_H^{LOD}|||_h \lesssim H$$

holds. The condition number scale as $\kappa \lesssim H^{-2}$.

Numerical verification – Fractal domain

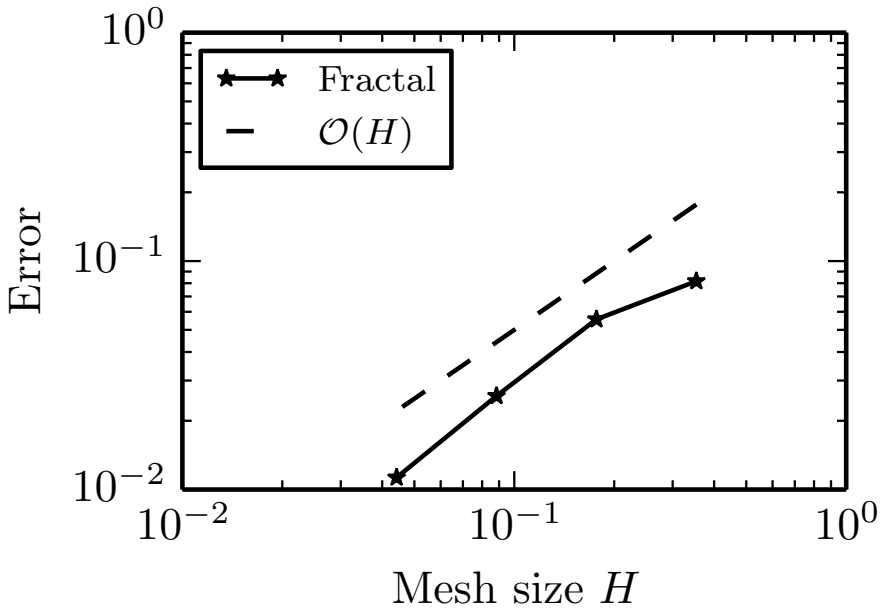
Consider the Poisson equation in the domain:

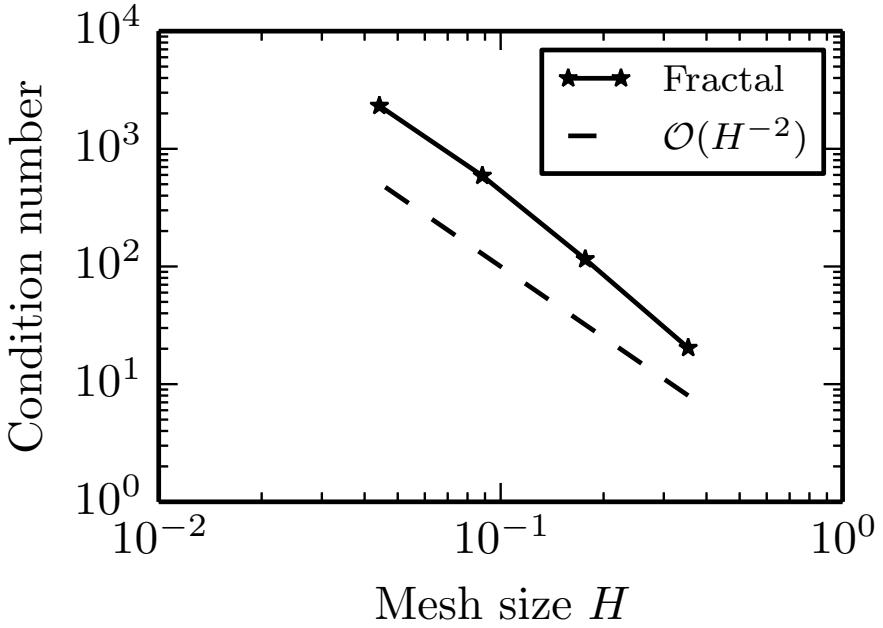


- Correctors are computed everywhere
- Mixed boundary condition

Numerical verification – Fractal domain

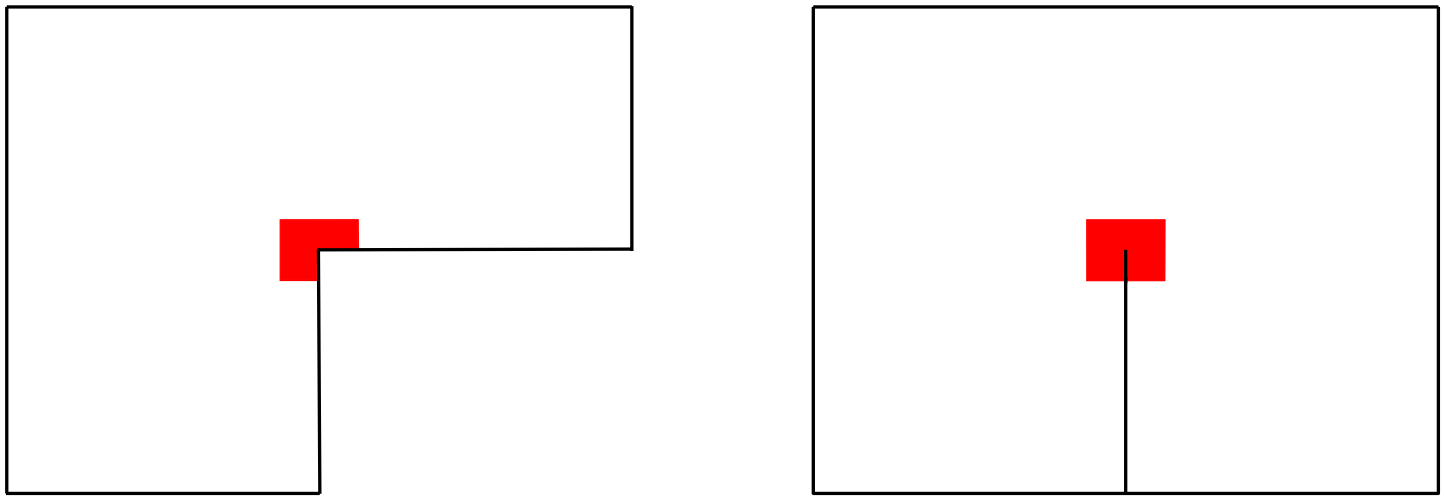
- The convergence in relative energy norm
- Conditioning





Numerical verification – Local singularities

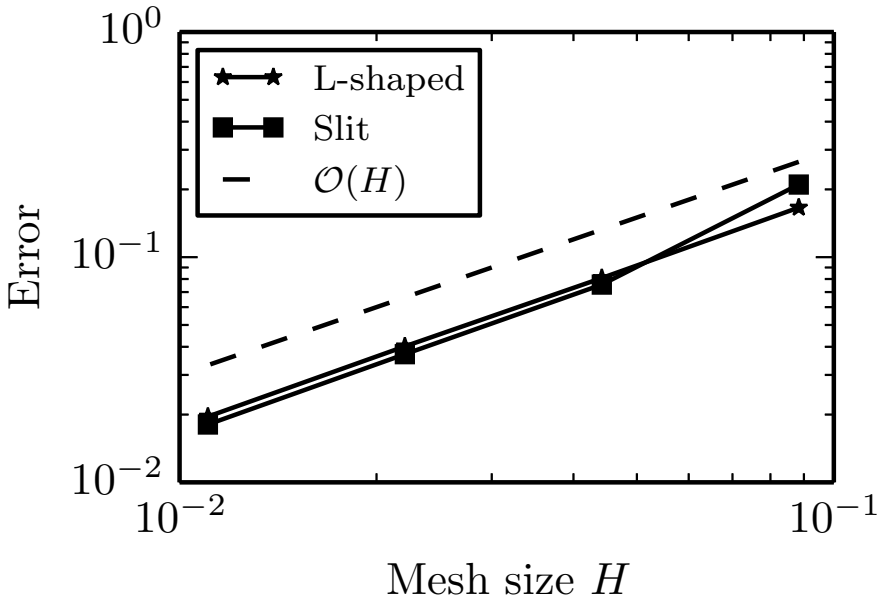
Consider the Poisson equation in the domains:

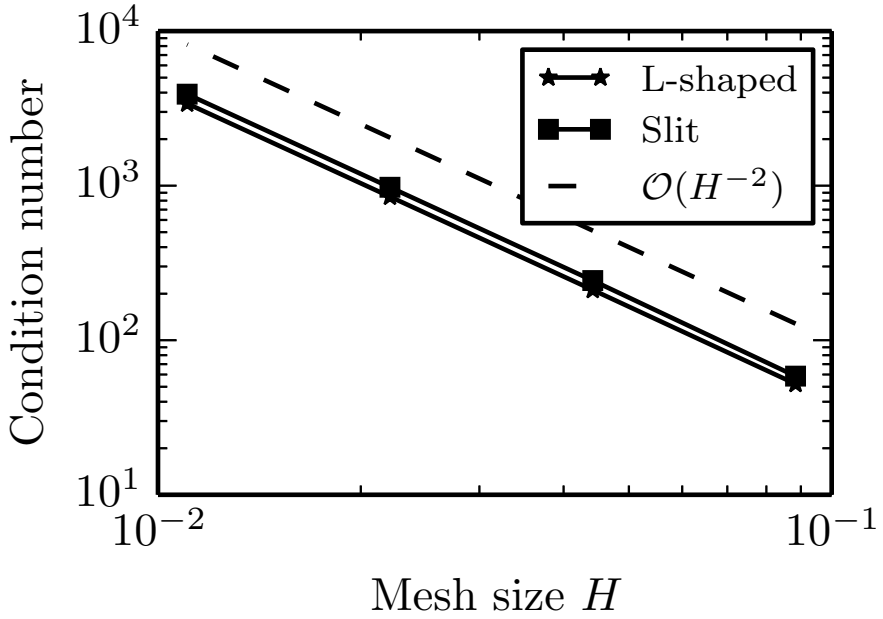


- Correctors are computed in the red areas
- Dirichlet boundary condition

Numerical verification – Local singularities

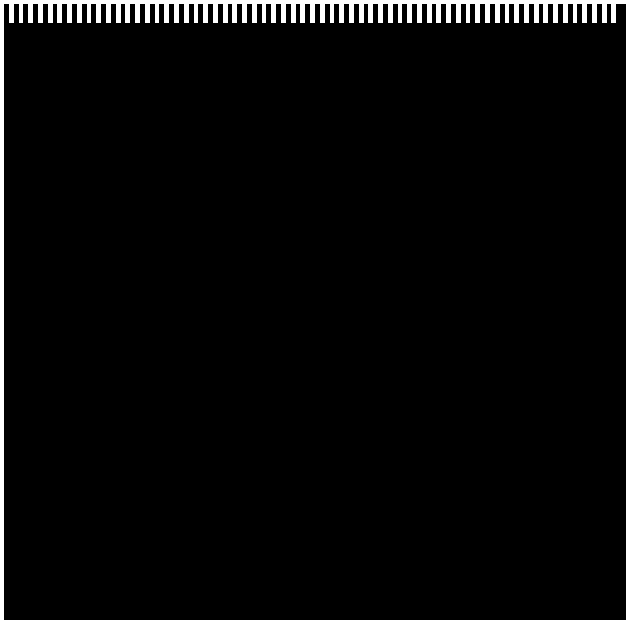
- The convergence in relative energy norm
- Conditioning

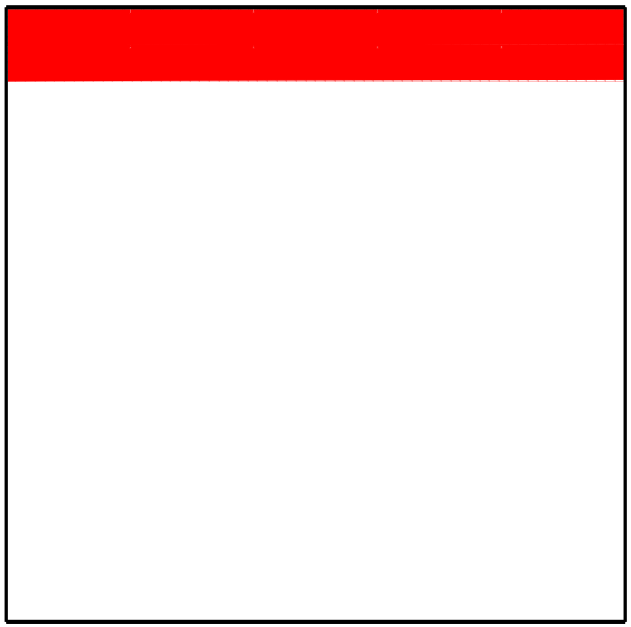




Numerical verification – Saw tooth boundary

Consider the Poisson equation in the domain:

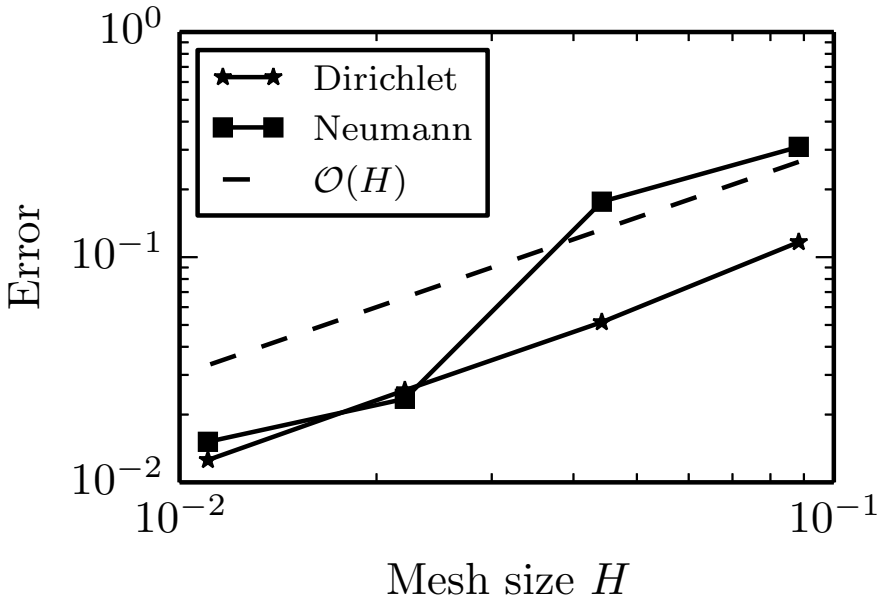


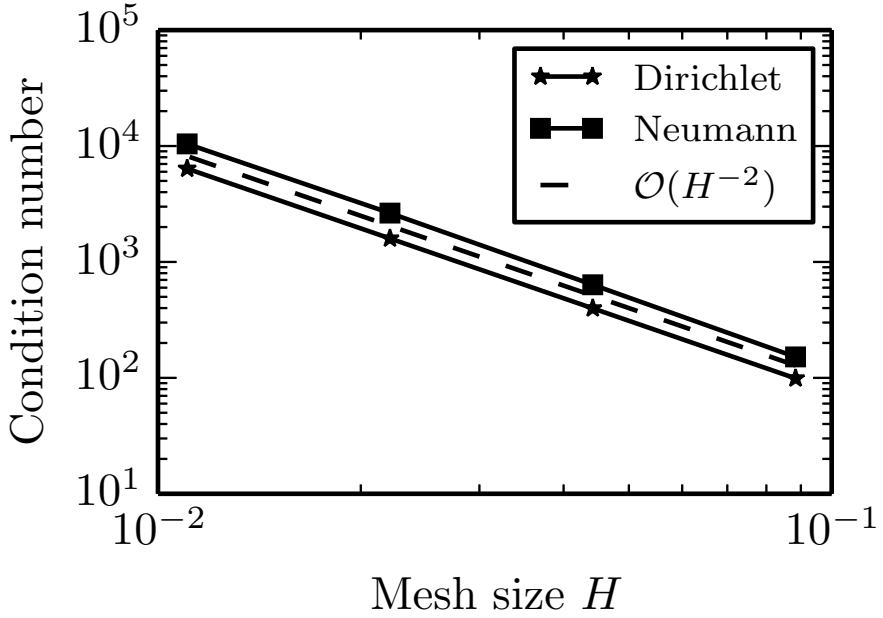


- Correctors are computed in the red area
- Test both Dirichlet and Neumann boundary condition on the saw tooth

Numerical verification – Saw tooth boundary

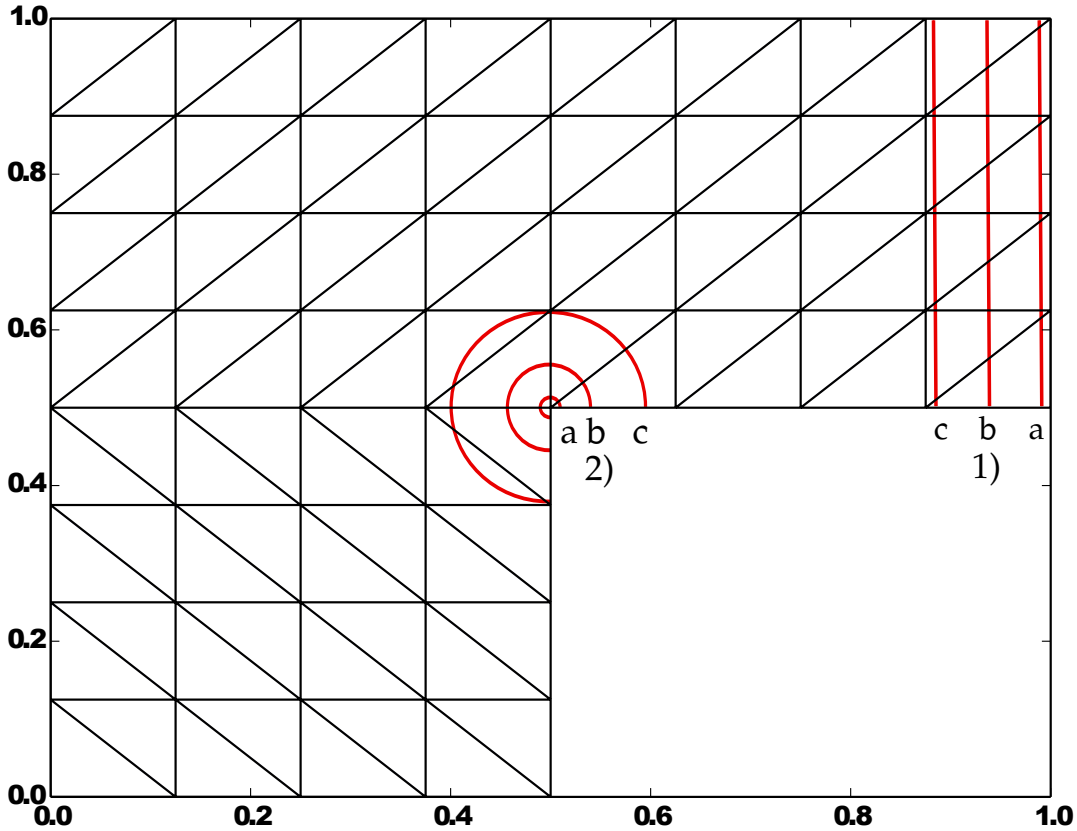
- The convergence in relative energy norm
- Conditioning





Numerical verification – Cut domain

Consider the Poisson equation in the domain:



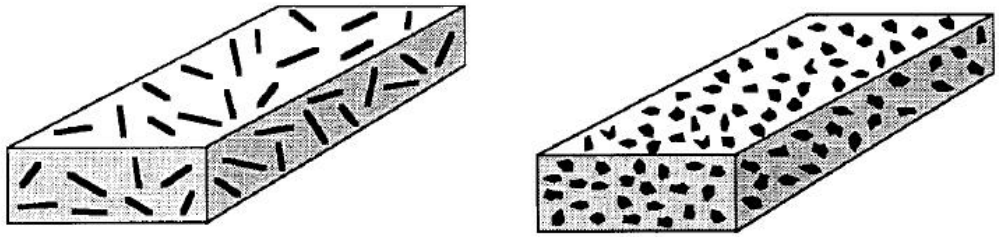
- Correctors are computed everywhere
- Conside a fix mesh and cut the domain in different ways

Numerical verification – Cut domain

Cut 1	$e_{\mathrm{rel}}(a)$	$e_{\mathrm{rel}}(b)$	$e_{\mathrm{rel}}(c)$
D	0.085	0.082	0.082
D-N	0.092	0.078	0.077
N-D	0.036	0.036	0.035
	$\mathrm{cond}(a)$	$\mathrm{cond}(b)$	$\mathrm{cond}(c)$
D	10.37	10.59	11.47
D-N	10.82	11.17	12.06
N-D	272.56	254.58	256.48

Cut 2	$e_{\mathrm{rel}}(a)$	$e_{\mathrm{rel}}(b)$	$e_{\mathrm{rel}}(c)$
D	0.086	0.091	0.100
D-N	0.086	0.081	0.080
N-D	0.037	0.052	0.068
	$\mathrm{cond}(a)$	$\mathrm{cond}(b)$	$\mathrm{cond}(c)$
D	10.32	10.08	9.49
D-N	10.41	11.98	13.56
N-D	222.78	99.95	71.06

Recent development and collaboration

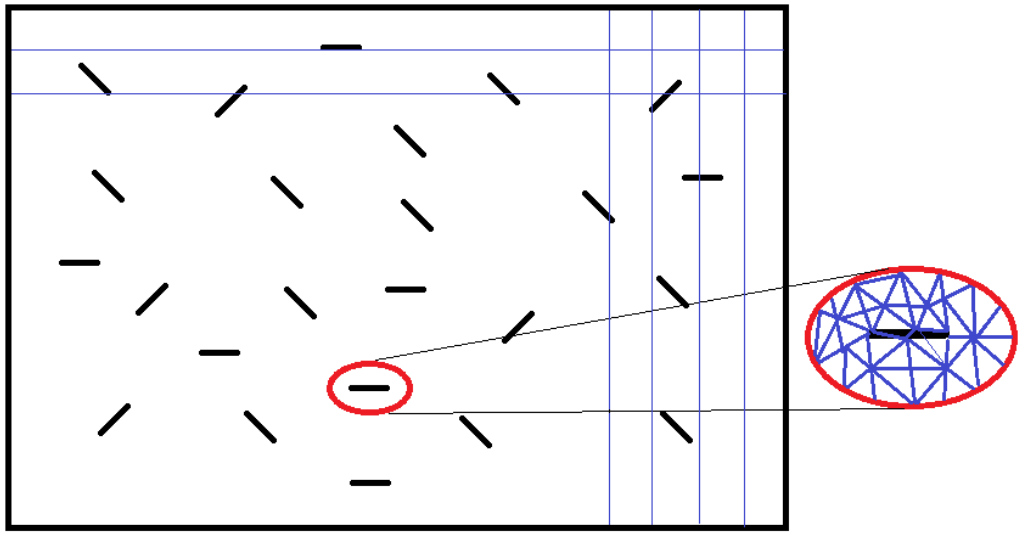


We consider a Poisson type model problem with a diffusion coefficient A that varies between two different values:

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

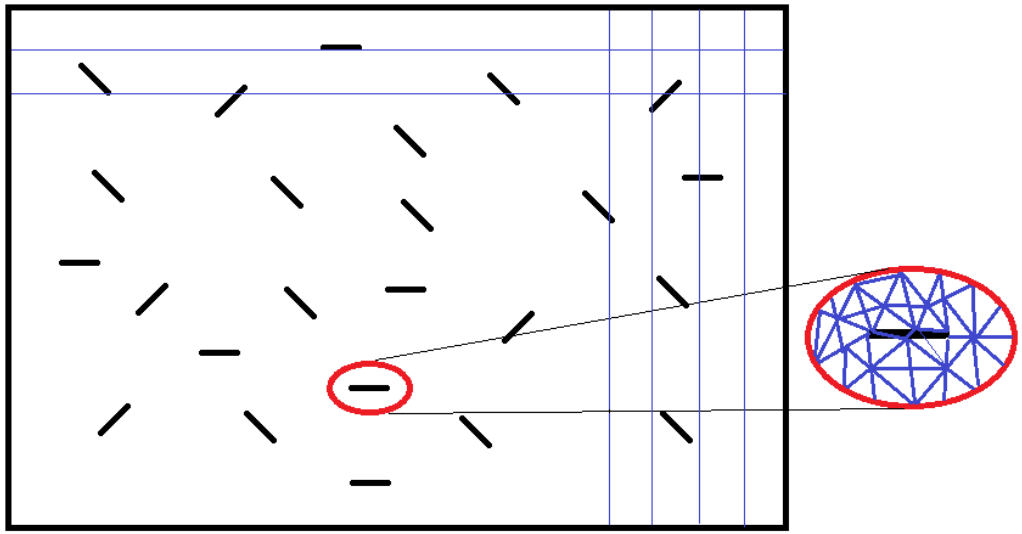
- The objects may be short fibres/particles or cracks/holes
- the solution has low regularity at the boundary of the objects
- local mesh refinement work for single configuration but not when multiple configurations or ”moving” objects are allowed
- Monte Carlo simulation or optimization procedure

Recent development



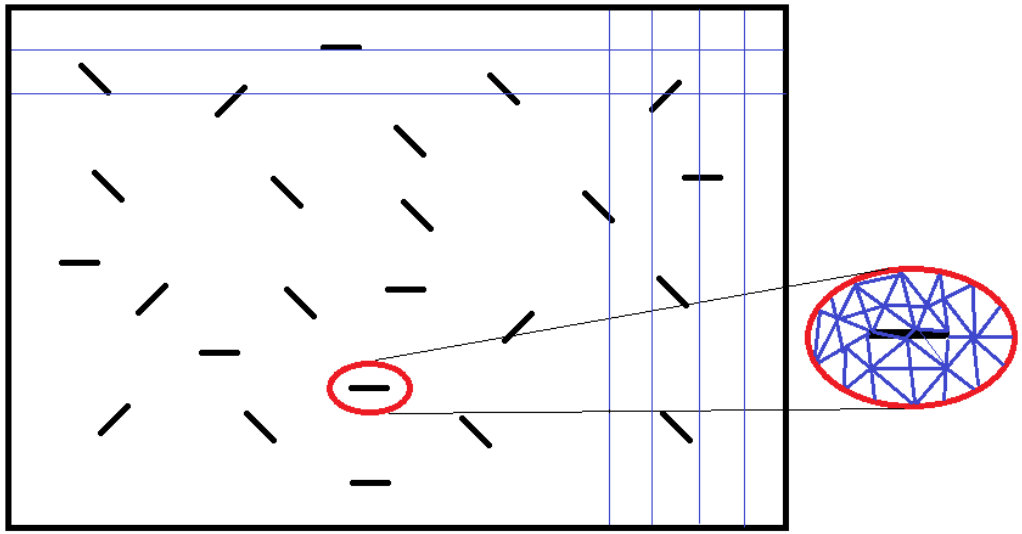
- In order to treat multiple configurations we want a regular static coarse background mesh.
- We only compute LOD basis functions in a region around each object and use standard P1 FEM basis functions in between.
- The size of the surrounding region can be controlled by H to meet tolerance, p adaptivity, DG. .
- If the regions overlap we compute basis functions for the union of the overlapping domains.

Recent development



- CutFEM allows us (we hope) to ”glue” the LOD computations to the background mesh avoiding remeshing.
- The assembly of the LOD parts is independent of the orientation of the object (rotation,translation).
- If the objects have the same shape huge savings are possible.
- Compared to CutFEM using spatially adapted subgrids around the objects the LOD approach leads to much smaller systems of equations for each configuration of the objects.

Recent development



- Random distribution of objects: Monte-Carlo simulation can be performed on the coarse scale with ”fine scale” accuracy.
- Design of materials: Optimization procedure where the objects are moved in order to minimize some output. Again repeated solves on the coarse scale still gives ”fine” scale accuracy.

Comments/questions/possible collaborations

- The problem is very similar to complex boundary, holes is a direct application.
- Any comments from or difficulties seen by the CutFEM experts?
- We got the idea from porous media flow applications, where there is a great uncertainty in the location and direction of defects. We seek applications in composite materials which fits our framework.
- Uncertainty quantification in material science is a possible application for this approach.
- What about applicability to optimal design problems?

We will start this work after the summer, in collaboration with Fredrik Hellman