Computational mathematics for heterogeneous materials

Axel Målqvist

Department of Mathematical Sciences
Chalmers University of Technology and University of Gothenburg

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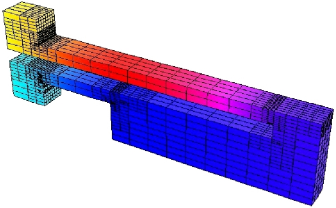
Partial differential equations (PDE)

Heat equation: $$\frac{\partial}{\partial t}u(x,t) - \sum_{i=1}^{3}\frac{\partial}{\partial x_i}\left(A(x)\frac{\partial u(x,t)}{\partial x_i}\right) = f(x,t)$$



Many physical processes are described mathematically by PDEs.

- Elasticity (structural mechanics, modal analysis)
- Electromagnetism (waves, Joule heating)
- Fluid flow (porous media, fluid-solid interaction)
- Quantum physics (wave function)

Why solve partial differential equations?

Industry:

- Simulation is cheaper than experiments
- Systematic way to optimize design

Government:

- Environment (climate, radioactive waste)
- Disasters (flood waves, hurricanes, nuclear disaster)

Science:

- Detailed understanding of physical processes
- Build intuition in mathematical analysis (conjecture)

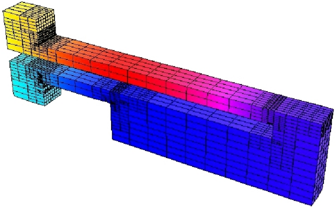
Mathematical analysis and numerical analysis

Mathematical analysis can give:

- Existence, uniqueness
- Properties such as conservation of mass or energy
- Regularity (smoothness) of the solution
- Restrictions on the data

Numerical analysis uses all this to:

- Develop efficient algorithms to solve the PDE
- Analyze the error due to finite precision

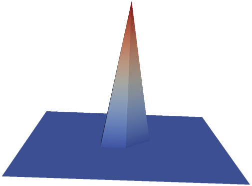


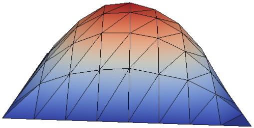
Finite element method

Stationary heat equation:

$$-\sum_{i=1}^{3} \frac{\partial}{\partial x_i}\left(A(x)\frac{\partial}{\partial x_i}u(x)\right) = f(x), \quad \text{in } \Omega.$$

with boundary condition $u_{\partial\Omega} = 0$. Let $V_h \subset V$ be space of continuous piecewise linear functions.





The finite element solution u_h is an approximation (projection) of the exact solution.

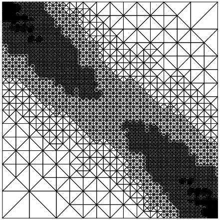
Accuracy and challenges

The error for smooth data fulfills,

$$\|u - u_h\| := \left(\int_\Omega |u - u_h|^2 \, dx \right)^{1/2} \leq Ch^2 \|f\|,$$

here h is mesh size. This does *not* hold if

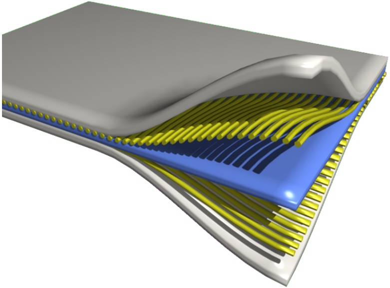
- Local roughness (corners, localized data f),



  Local roughness is treated by adaptive mesh refinement.

- Global roughness (rough material data A).

Heterogeneous materials



Porous media flow

Composites

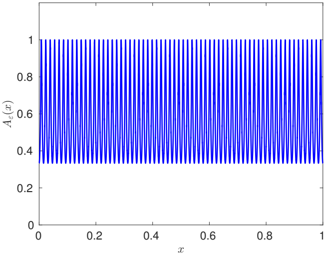
Simple 1D example of how FEM fails

Example (periodic coefficient):

We consider

$$-\frac{d}{dx}\left(A(x)\frac{d}{dx}u(x)\right) = 1, \quad u(0) = u(1) = 0,$$

with $A(x) = (2 + \cos(2\pi x/\varepsilon))^{-1}$, where $\varepsilon = 2^{-6}$.



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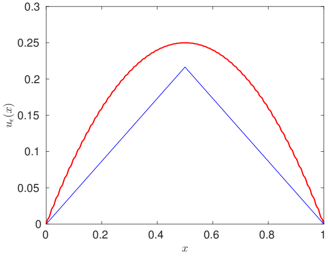

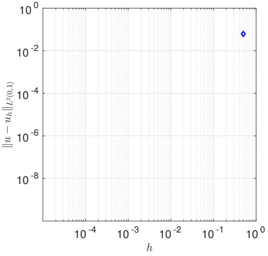

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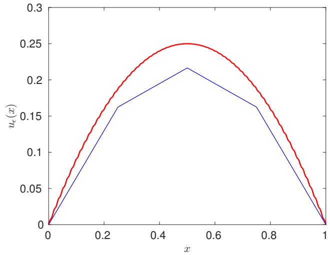
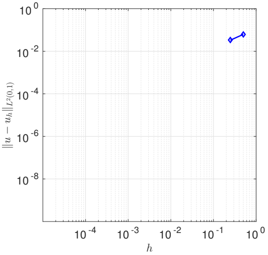


solution and P1-FEM-approximation



$L^2(\Omega)$ – error vs. h

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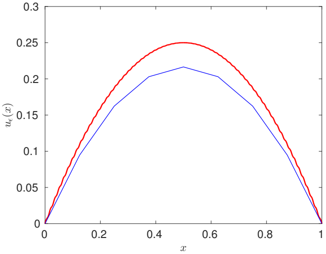

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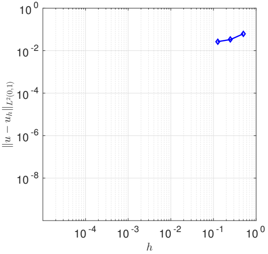

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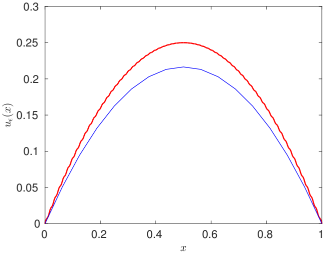

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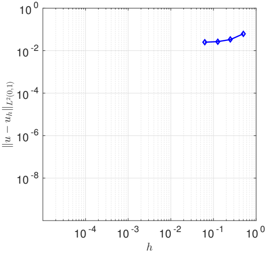

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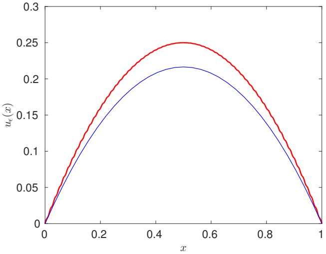

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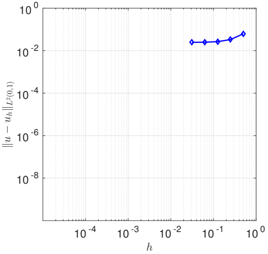

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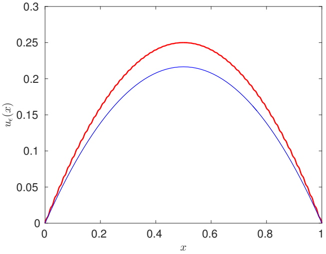

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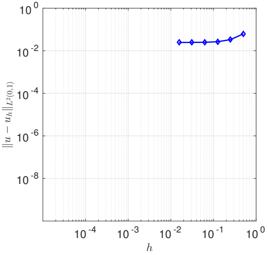

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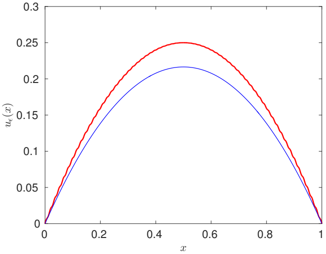

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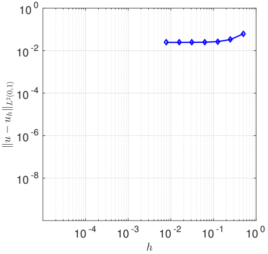

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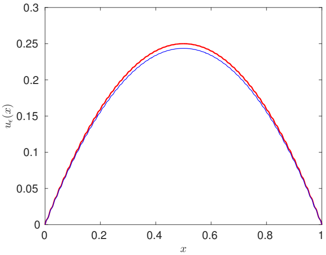

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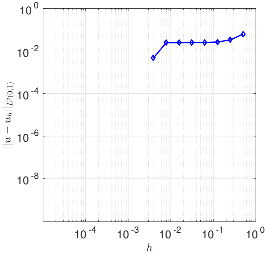

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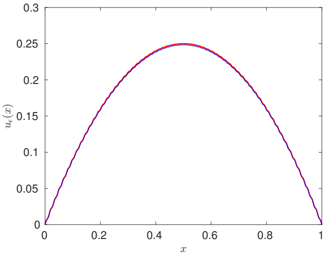

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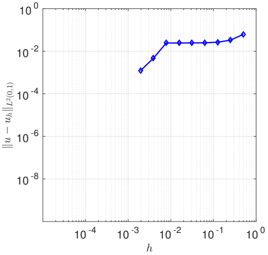

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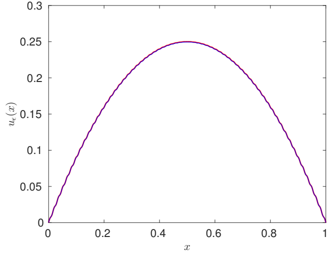

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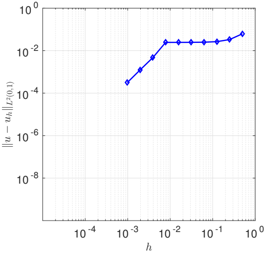

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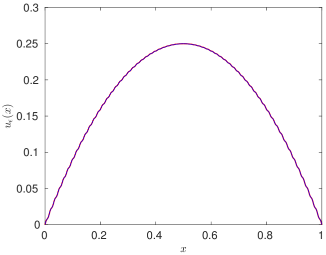

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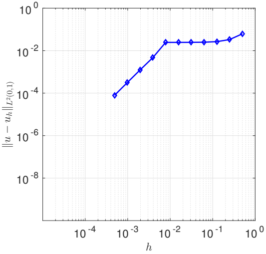

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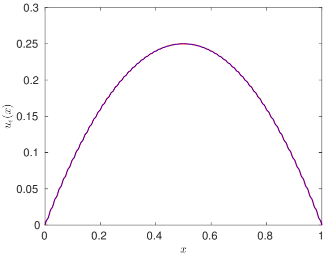

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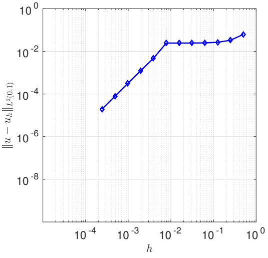

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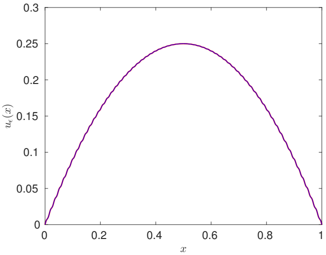

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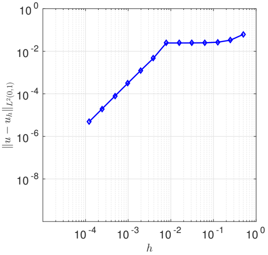

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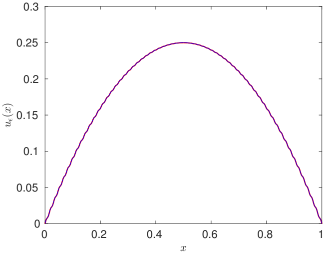

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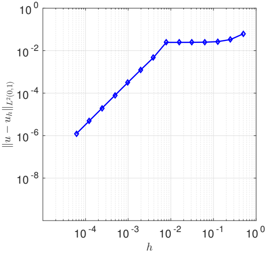

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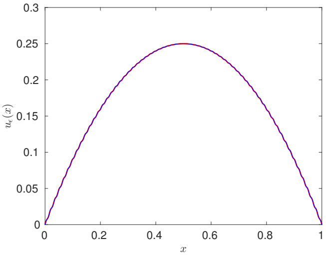

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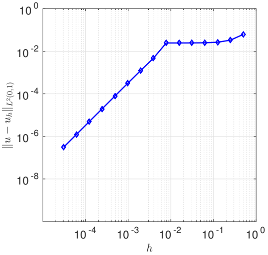

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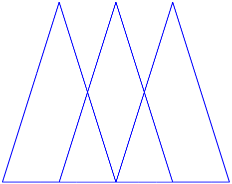
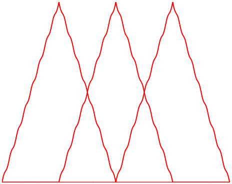
Resolution using two scale basis functions

In 1D one can construct two scale basis functions

$$\tilde{\Lambda}_j(x) := \begin{cases} \dfrac{\int_{x_{j-1}}^{x} A^{-1}(s)\, ds}{\int_{x_{j-1}}^{x_j} A^{-1}(s)\, ds}, & \text{if } x \in [x_{j-1}, x_j], \\ 1 - \dfrac{\int_{x_j}^{x} A^{-1}(s)\, ds}{\int_{x_j}^{x_{j+1}} A^{-1}(s)\, ds}, & \text{if } x \in [x_j, x_{j+1}], \\ 0, & \text{else.} \end{cases}$$





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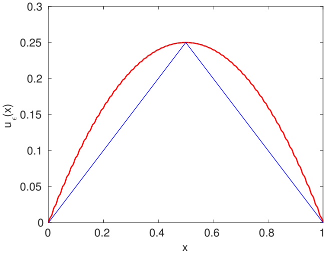

We plot $I_h \tilde{u}_h$ which in fact is exact in the nodes.

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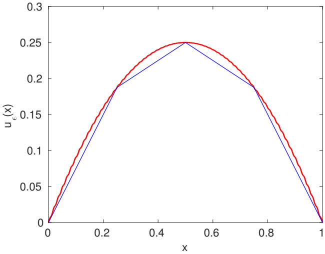

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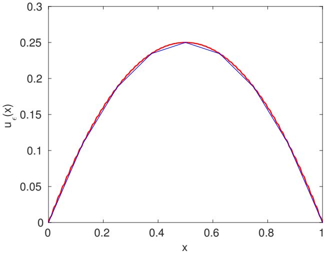

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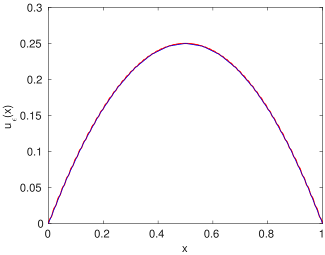

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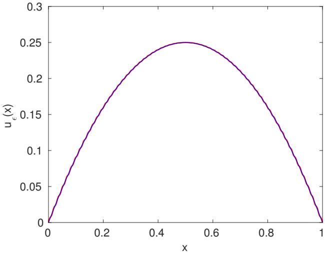
$$\tilde{\Lambda}_j(x) := \begin{cases} \dfrac{\int_{x_{j-1}}^{x} A^{-1}(s)\,ds}{\int_{x_{j-1}}^{x_j} A^{-1}(s)\,ds}, & \text{if } x \in [x_{j-1}, x_j], \\ 1 - \dfrac{\int_{x_j}^{x} A^{-1}(s)\,ds}{\int_{x_j}^{x_{j+1}} A^{-1}(s)\,ds}, & \text{if } x \in [x_j, x_{j+1}], \\ 0, & \text{else.} \end{cases}$$



We plot $I_h \tilde{u}_h$ which in fact is exact in the nodes.

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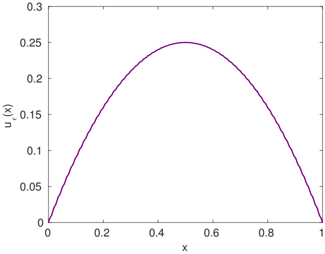

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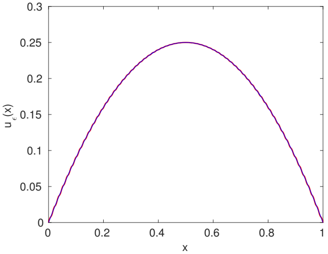

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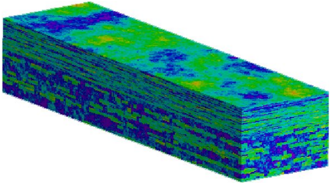
Generalization to higher dimensions



- Resolving all scales with FEM is often too expensive
- No simple formula for $\tilde{\Lambda}_j$ available
- Classical results only for periodic coefficients (homogenization theory)

My goal has been to construct optimal basis $\tilde{\Lambda}_j$ without assuming periodicity (in 2D, 3D).

Generalization to higher dimensions

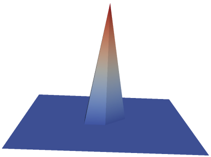
Poisson's equation on weak form: find $u \in V$ such that

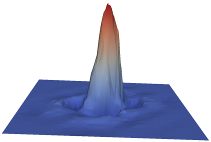
$$a(u, v) := (A\nabla u, \nabla v) = (f, v), \quad v \in V.$$

Let $V = \tilde{V}_h \oplus V^f$ where $V^f = \{v \in V : I_h v = 0\}$ and $\tilde{V}_h = \{v \in V : a(v, w) = 0, \quad \forall w \in V^f\}$. Let $\tilde{u}_h \in \tilde{V}_h$ solve

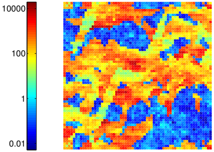
$$a(\tilde{u}_h, v) = (f, v) = a(u, v), \quad v \in \tilde{V}_h.$$

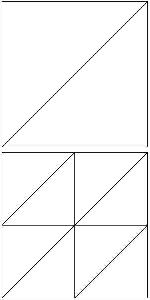
Then $I_h(u - \tilde{u}_h) = 0$ and furthermore $\|u - \tilde{u}_h\| \leq Ch^2 \|f\|$.





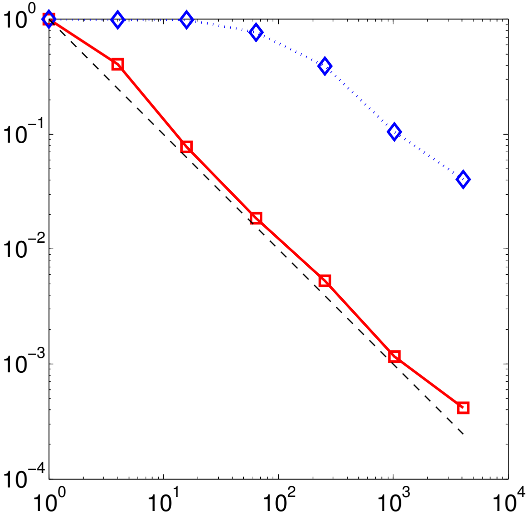
Numerical experiment: Poisson's equation





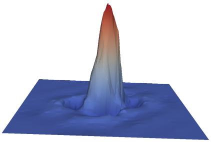
$h = 2^{-1}, 2^{-2}, \dots, 2^{-7}$

$h_{\text{ref}} = 2^{-9}$, $\ell = \log(1/h)$



$\|u_{h_{\text{ref}}} - \tilde{u}_h\|$ vs. #dof

Mathematical challenges



- Prove exponential decay of basis
- High contrast data, channels, interpolation
- Prove a priori error bound independent of variations in A
- Extend theory to problems relevant in applications (time dependent, nonlinear, systems)

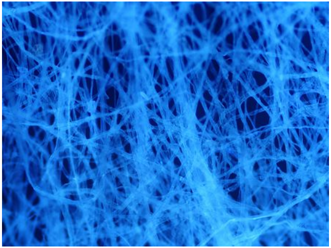
A. Persson, Numerical Analysis of Evolution Problems in Multiphysics, 2018.

Recent developments

Several groups continues to develop this methodology (2014–present)

- Göteborg (time dependent, network models, high contrast data)
- Augsburg (Helmholtz, stochastic, quantum physics)
- Stockholm (Elasticity, quantum physics)
- Münster (Helmholtz, RBM)
- Berlin (iterative solvers)
- Lusanne (Wave)
- Heidelberg (High contrast data)
- Laramie (WY) (porous media flow)
- Athens (Discontinuous Galerkin)

Future work



- Mechanical properties of paper (Fraunhofer)
- Random defects in materials
- Interface models for cracks, reinforcements